FINITE ELEMENT SIMULATION OF POLLUTANT TRANSPORT IN AQUIFERS

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by

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CERTIFICATE

This is to certify that the thesis entitled "Finite Element Simulation of Pollutant Transport in Aquifers" submitted by Shri Pramod Kumar Singh in partial fulfilment of requirements for the degree of Master of Technology at Indian Institute of Technology Kanpur is a record of bonafide research work carried out by him under my supervision and guidance. The work embodied in this thesis has not been submitted elsewhere for a degree.

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- P.K. Singh

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NOTATIONS

c	concentration of dispersing mass in liquid phase i.e. mass of pollutant per unit volume of solution (mg/l)
c^*	concentration of source fluid (mg/l)
D_{ij}	hydrodynamic dispersion tensor (m^2/min)
D_L	ongitudinal dispersion coefficient (m^2/min)
D_m	coefficient of molecular diffusion (m^2/min)
D_t	coefficient of turbulent diffusion (m^2/min)
D_T	transverse dispersion coefficient (m^2/min)
n	porosity of porous media i.e. aquifer
q	volumetric fluid injection rate at the source per unit volume of medium (min^{-1})
R	retardation factor
S	the mass of pollutant adsorbed per unit volume of media (mg/l)
t	the time (min)
u_i	the component of Darcy's velocity vector in i^{th} direction (m/min)
α_L	longitudinal dispersivity (m)
α_T	transverse dispersivity (m)
α	flux at seepage boundary (mg/l per meter)
λ	radioactive decay coefficient equal to reciprocal of mean life time of radioactive pollutant (min^{-1})
ϕ	values of nodal concentration
β	width of domain.

ABSTRACT

In the present study an attempt has been made to study the pollutant transport in groundwater flowing through aquifers. A suitable mathematical model has been developed to predict the spread of pollutant in groundwater. This model incorporates many different methods of pollutant transport like mechanical dispersion molecular diffusion, hydrodynamic dispersion etc. and other phenomena such as adsorption, radioactive decay etc.

The resulting differential equations describing pollutant transport have been solved for various boundary conditions and other parameters in both - one and two dimensional, cases using finite element method. It is seen that numerical solution and the analytical results match closely for some special case. It is also seen that for radioactive elements with higher half life period the effect of radioactive decay on pollutant concentration is not significant. Also the volumetric fluid injection rate and its pollutant concentration affects the concentration profile even at a distance far away from the source. For two dimensional cases the dispersion equation has been solved for two different sets of boundary conditions, and the concentration contours for one set of boundary conditions are presented.

CHAPTER 1

INTRODUCTION

1.1. General:

Water resources engineer is often concerned with proper management and effective use of groundwater. It is important for such a person to be able to predict the changes in a system due to any proposed policy and thus obtain the new state of the system, given the initial system. Such a prediction before hand helps in checking the feasibility of the system and also having knowledge before hand about any ill effects that it may cause. Also such prediction helps in choosing from several options, the best policy according to some criteria. For example in a groundwater system it should be possible to predict water levels, salinity, spring discharges, land subsidences etc., which are the system state variables which may change due to any proposed policy like pumping, artificial recharge etc.

In many regions groundwater does not pose major biological problem or physical quality problem, but in certain cases the presence of faulty sewage pipes, oil spillage etc. may cause severe pollution of groundwater. Pollutants, thus introduced into groundwater, may travel large distances in an aquifer and thus pollute groundwater over a large area. Also groundwater is liable to pick up minerals while passing through rocks, containing such minerals. This may lead to deterioration of groundwater quality. Another problem is that of salinity. Most groundwaters

becomes salinised by pollutants broughtdown from the surface. In natural condition an equilibrium is reached between water leaving the formation and pollutants carried with it. But due to activities like groundwater recharge, water of inferior quality is introduced, then the pollutant concentration in the groundwater increases and this leads to increase in salinity.

1.2. Objective of Study:

Groundwater quality problem in water resources engineering involves the mass transport in porous media where 'mass' is some pollutant moving with water in the voids of soil both in saturated and unsaturated zones. The mechanism which affect the transport of pollutant are convection, mechanical dispersion, molecular diffusion, solute pollutant interaction, various chemical reactions and radioactive decay phenomenon.

In the present work the laws governing the movement and accumulation of pollutants in groundwater flow have been studied. The movement of pollutant has been described using partial differential equations subjected to initial and boundary conditions. These equations have then been solved by finite element method which is a very powerful technique. The solution of such equations enable the engineer to predict the distribution of pollutants in the aquifer.

1.3. Significance of Study:

A major problem, which is of interest in development and management of water resources system, is that of water quality.

In fact, with increased demand for water in most parts of world and intensification of water utilisation, the quality problem becomes the limiting factor in development of water resources in many parts of world. Although in such regions, the quality of both surface and groundwater resources deteriorates as a result of pollution, special attention should be devoted to the pollution of groundwater in an aquifer due to their very slow velocity. Hence, although it seems that groundwater is more protected than surface water against pollution, it is still subjected to pollution and when latter occurs, the restoration to original, non-pollutated state, is more difficult (Bear, 1972).

1.4. Scope of Study:

In the present work the aquifer considered is saturated, porous medium. The effects of convection, hydrodynamic dispersion, adsorption and radioactive decay on pollutants are considered in one dimensional and two dimensional flow fields. In one dimensional case linear and quadratic elements have been taken. Solutions of two dimensional dispersion equation with different boundary conditions have been presented. Programs have been developed for F.E.M. solution of one (for linear and quadratic cases) and two dimensional cases.

1.5. Organisation of Report:

The study is reported in five chapters. The sequence of the topics discussed along with a brief description of each chapter is given below.

In Chapter 2 the work done previously in this field is reported. This discussion mainly consists of a chronological report of the various attempts that were made at mathematical modeling of pollutant transport in groundwater using finite element method of solution.

In Chapter 3 a brief qualitative review of the various processes of pollutant transport in groundwater has been given, followed by the governing partial differential equation which describes the transport both in one dimensional and two dimensional flow fields. Then the finite element formulation of the above equations have been given.

In Chapter 4 the results obtained by solving the partial differential equations subjected to various boundary conditions by the finite element method, have been described in detail. In one dimensional case results obtained by the finite element method have been compared with the results obtained analytically in one special case. Two dimensional problem has also been solved. The results have been presented in tabular and graphical forms.

In the last chapter a brief summary of the work has been given with suggestions for future work.

CHAPTER 2

LITERATURE REVIEW

In the field of groundwater management, the prediction of groundwater quality by using mathematical model warrants special attention. Several attempts have been made in the past for developing suitable mathematical models to predict pollutant transport in groundwater. A brief review of the work done in this field is presented in the following paragraphs.

Pinder (1973) had simulated the movement of groundwater by Galerkin method of approximation in connection with finite element method of analysis. In solving the groundwater flow and mass transport equations through this approach, he had used functional representation of dispersion tensor, transmissivity tensor and fluid velocity as well as an accurate representation of boundaries of irregular geometry.

Nishi et.al. (1976) considered the hydrodynamic dispersion in seepage from a triangular channel. In this they employed isoparametric elements to solve the two dimensional convection-dispersion problem. He made a comparison between finite element and finite difference solutions to this problem.

Narsimhan et.al. (1978) developed mixed implicit-explicit Galerkin finite element method which was ideally suited for a wide class of problems arising in subsurface hydrology. These problem include confined saturated flow, unconfined flow under

free conditions subjected to Dupuit's assumption and flow in aquifers which are partly confined and partly unconfined.

Lindorff (1979) studied the severity and extent of groundwater contamination. According to him the severity and extent of groundwater contamination is determined by (1) hydrogeologic setting, (2) nature of contaminant and (3) effectiveness of regulatory action.

Grove and Wood (1979) tried to predict and verify the subsurface water quality changes during artificial recharge.

Noorishad and Mehran (1982) obtained the two dimensional transient dispersive-convective transport of nonconservative solute species in porous media. They developed a two nodal point, one dimensional, transport element for fractures which provides a number of advantages relative to conventional fracture representation of two dimensional continuum elements.

Cooley (1983) presented some new procedures for forming numerical solutions of saturated flow problems. The techniques for addressing the problems, controlling the stability of nonlinear equation solver, devising a reliable, yet efficient method for determining the position of seepage surface, have been applied in subdomain of finite element discretization of the governing flow equations. He presented the solutions of problems like (a) steady state flow through square embankment, (b) steady state flow to a well, (c) drainage from a square block, (d) drainage involving multiple seepage faces, (e) one dimensional vertical infiltration, (f) transient seepage from stream and (g) steady state groundwater flow around lakes.

Huykorn et.al. (1984) developed a Galerkin finite element formulation for the numerical solution of water flow in saturated soil systems. He included a solution strategy based on Picard and Newton algorithm. Both algorithms are formulated for both rectangular and triangular elements. In this a comparative study of Picard and Newton-Raphson algorithm is provided. Four examples are presented to demonstrate the effectiveness of the finite element approach. These examples show that the nonlinear solution schemes are capable of accommodating cases involving larger variations in saturated hydraulic conductivity as well as highly nonlinear soil moisture characteristics.

Yang (1988) conducted a two dimensional saturated-unsaturated water and solute transport experiment in a soil tank infiltration and drainage condition. In this, a model accounting for mobile and immobile water phases is used to describe the solute transport. A Galerkin finite element model is designed to solve the transient movement of water in saturated-unsaturated soil. The seepage velocities at nodal points are obtained by using the same finite element as for the pressure field.

CHAPTER 3

MATHEMATICAL PROBLEM FORMULATION

3.1. General:

Pollutant is a term used to denote dissolved matter carried with the groundwater and accumalating in the aquifer. For groundwater pollution study, water resources engineer must be familiar with potential sources of groundwater pollution, extent of groundwater pollution and remedial measures to be taken in order to rectify the effects of such pollution.

The major sources of groundwater contamination are given in Table 1.

After identifying the sources of groundwater pollution, the extent of such pollution must be determined. To predict this extent the mass transport of pollutant in groundwater must be studied. Several mathematical models have been described, that simulate pollutant transport in aquifer. The phenomena of pollutant transport have been described in the following sections.

3.1.1. Mechanical Dispersion:

As the flow takes place, pollutant gradually spreads and occupies larger portion of flow domain. This spreading is in both longitudinal direction, namely that of the average flow, and in the direction transverse to the average flow. This spreading caused by velocity variations at the microscopic level is known as mechanical dispersion or convective diffûsion.

TABLE 1. CLASSIFICATION OF SOURCES OF GROUNDWATER CONTAMINATION (Lindorff, 1979)

Wastes		Non-wastes
Sources designed to discharge to land and groundwater	Sources that may discharge waste to land and groundwater unintentionally	Source that may discharge a contaminant (not a waste) to land and groundwater
1) Spray irrigation	1) Surface impoundments	1) Buried products, storage tanks and pipe lines
2) Septic systems, cesspools etc.	2) Land fills	2) Accidental spills
3) Land disposal of sludge	3) Animal feed lots	3) Ore stock piles
4) Infiltration or percolation basins	4) Acid mine drainage	4) Application of highway salt
5) Waste disposal wells	5) Mine spoil pipes	5) Product storage ponds
6) Brine injection wells		6) Agricultural activities

3.1.2. Molecular Diffusion:

An additional mass transport phenomenon occurs simultaneously with mechanical dispersion. This occurs due to variations in pollutant concentration within the liquid phase. This is caused by molecular diffusion. This molecular diffusion is of two types.

3.1.2.1. Ordinary Molecular Diffusion: When a fluid is considered as continuum, the velocity of small fluid element is defined as the ratio of total momentum (vector) of its molecules to their mass. Actually, in addition to this velocity, the molecules in this element have random motion. For example, a fluid element is said to be 'at rest' if its centre of mass remains stationary (i.e. if the total momentum of its molecules is zero), although the molecules are moving randomly in various directions. As a result of the random motion, molecules of certain material in high concentration at one point will spread with time even in fluid 'at rest'. This net molecular motion from a point of higher concentration to one of lower concentration is called ordinary molecular diffusion.

3.1.2.2. Turbulent Diffusion: Fluid flows in nature are usually turbulent. The velocity at a point in such a flow fluctuates randomly in direction and in magnitude. A turbulent flow is often imagined to be a main flow with numerous eddies of various size.

When a turbulent flow is described with the temporal mean velocity $\bar{q}$ and the temporal mean concentration $\bar{c}$ at each point, the diffusion equation for dilute solution is

$$\frac{\partial \bar{c}}{\partial t} + \bar{q} \cdot \nabla \bar{c} = D_m \nabla^2 \bar{c} + \nabla \cdot (D_t \nabla \bar{c}) \quad (3.1)$$

where D_t = coefficient of turbulent diffusion or eddy diffusion

and D_m = coefficient of molecular diffusion.

Usually $D_t \gg D_m$ and the term D_m can be neglected. In a channel, the turbulence is anisotropic, especially near the solid boundary. For anisotropic turbulence, D_t is not a scalar quantity and is often assumed to be a second rank tensor, with nine component D_{ij}

$$\begin{aligned}\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial y} + \bar{w}\frac{\partial \bar{c}}{\partial z} &= \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial \bar{c}}{\partial x} + D_{xy}\frac{\partial \bar{c}}{\partial y} + D_{xz}\frac{\partial \bar{c}}{\partial z}\right) \\ &+ \frac{\partial}{\partial y}\left(D_{yx}\frac{\partial \bar{c}}{\partial x} + D_{yy}\frac{\partial \bar{c}}{\partial y} + D_{yz}\frac{\partial \bar{c}}{\partial z}\right) \\ &+ \frac{\partial}{\partial z}\left(D_{zx}\frac{\partial \bar{c}}{\partial x} + D_{zy}\frac{\partial \bar{c}}{\partial y} + D_{zz}\frac{\partial \bar{c}}{\partial z}\right) \quad (3.2)\end{aligned}$$

The components D_{ij} vary from point to point in a flow. For an isotropic turbulent flow, $D_{xx} = D_{yy} = D_{zz}$ and other D_{ij} are zero (i.e. $D_{xy} = D_{yx} = D_{yz} = D_{zy} = D_{xz} = D_{xz} = 0$).

3.1.3. Hydrodynamic Dispersion:

This term denotes the spreading (at the macroscopic level) resulting from both mechanical dispersion and molecular diffusion. Molecular diffusion alone does take place also in absence of motion. Because molecular diffusion depends upon time its effect on overall dispersion will be more significant at low velocities. It is molecular diffusion which makes the phenomenon of hydrodynamic dispersion in purely laminar flow irreversible.

3.2. Basic Differential Equations:

The basic differential equation describing the process of transport of pollutant in a saturated porous medium, and accounting for the effects of convection, hydrodynamic dispersion, adsorption and radioactive decay can be expressed in its most general form as (derivation is in Appendix A)

$$n \frac{\partial c}{\partial t} + (1-n) \frac{\partial s}{\partial t} = \frac{\partial}{\partial x_i} \left[n D_{ij} \frac{\partial c}{\partial x_j} - u_i c\right] - \lambda[nc + (1-n)s] + qc^* \tag{3.3}$$

in which

c = concentration of dispersing mass in liquid phase i.e. the mass of solute per unit volume of solution (ML^{-3})

s = concentration of dispersing mass in solid phase i.e. the mass of solute adsorbed per unit volume of porous media (ML^{-3})

n = porosity of the porous media i.e. pore volume per unit volume of porous media (L^{o})

D_{ij} = hydrodynamic dispersion tensor (L^2T^{-1})

u_i = the component of Darcy's velocity vector in the i^{th} direction (LT^{-1})

λ = radioactive decay coefficient equal to reciprocal of mean life time of radioactive solute tracer (T^{-1})

q = volumetric fluid injection rate at the source per unit volume of medium (T^{-1})

c^* = concentration of source fluid

t = time (T)

x_i, x_j = the spatial co-ordinates (L)

Assuming a linear equilibrium adsorption, concentration of solid phase can be expressed as

$$s = kc \tag{3.4}$$

where k is constant.

With this assumption, equation (3.3) takes the following form

$$n \frac{\partial c}{\partial t} + (1-n)k \frac{\partial c}{\partial t} = \frac{\partial}{\partial x_i} [n D_{ij} \frac{\partial c}{\partial x_j} - u_i c] - \lambda[nc + (1-n)kc] + qc^*$$

or

$$n \frac{\partial c}{\partial t}[1 + \frac{(1-n)k}{n}] = \frac{\partial}{\partial x_i} [n D_{ij} \frac{\partial c}{\partial x_j} - u_i c] - \lambda nc [1 + \frac{(1-n)k}{n}] + qc^* \tag{3.5}$$

the term $(1 + k \frac{1-n}{n})$ in equation (3.5) is constant for given porous media and is known as the Retardation Factor. Thus equation (3.5) becomes

$$R \frac{\partial c}{\partial t} = \frac{\partial}{\partial x_i} [D_{ij} \frac{\partial c}{\partial x_j} - \frac{u_i}{n} c] - \lambda Rc + \frac{qc^*}{n}$$

or
$$R \frac{\partial c}{\partial t} - \frac{\partial}{\partial x_i} [D_{ij} \frac{\partial c}{\partial x_j} - \frac{u_i}{n} c] + \lambda Rc - \frac{q}{n} c^* = 0 \tag{3.6}$$

Equation (3.6) is the general form of equation describing the process of pollutant transport.

For Cartesian co-ordinates system, the above equation can be written in an expanded form for the case of one dimensional, two dimensional and three dimensional dispersions as shown below.

(i) <u>One dimensional dispersion in one dimensional flow field</u>

$$R \frac{\partial c}{\partial t} - D_{xx} \frac{\partial^2 c}{\partial x^2} + \frac{1}{n} \frac{\partial}{\partial x} (u_x c) + \lambda Rc - \frac{q}{n} c^* = 0 \tag{3.7}$$

(ii) Two dimensional dispersion in two dimensional field

$$R \frac{\partial c}{\partial t} - \left[D_{xx} \frac{\partial^2 c}{\partial x^2} + D_{xy} \frac{\partial^2 c}{\partial x \partial y} + D_{yx} \frac{\partial^2 c}{\partial y \partial x} + D_{yy} \frac{\partial^2 c}{\partial y^2}\right]$$

$$+ \frac{1}{n}\left[\frac{\partial}{\partial x}(u_x c) + \frac{\partial}{\partial y}(u_y c)\right] + \lambda R c - \frac{q}{n} c^* = 0 \qquad (3.8)$$

(iii) Three dimensional dispersion in three dimensional flow field

$$R \frac{\partial c}{\partial t} - \left[D_{xx} \frac{\partial^2 c}{\partial x^2} + D_{xy} \frac{\partial^2 c}{\partial x \partial y} + D_{xz} \frac{\partial^2 c}{\partial x \partial z} + D_{yx} \frac{\partial^2 c}{\partial y \partial x} + D_{yy} \frac{\partial^2 c}{\partial y^2}\right.$$

$$\left. + D_{yz} \frac{\partial^2 c}{\partial y \partial z} + D_{zx} \frac{\partial^2 c}{\partial z \partial x} + D_{zy} \frac{\partial^2 c}{\partial z \partial y} + D_{zz} \frac{\partial^2 c}{\partial z^2}\right]$$

$$+ \frac{1}{n}\left[\frac{\partial}{\partial x}(u_x c) + \frac{\partial}{\partial y}(u_y c) + \frac{\partial}{\partial z}(u_z c)\right] + \lambda R c - \frac{q}{n} c^* = 0 \qquad (3.9)$$

While writing the equations in the above forms, the components of dispersion tensor are treated constant, an assumption which is valid for homogeneous and isotropic porous media. The components of dispersion tensor for isotropic porous media can be worked out in terms of dispersivity and Darcy velocity components, as per following equations (Bear, 1972)

$$D_{xx} = D_L \frac{u_x^2}{|u|^2} + D_T \frac{u_y^2}{|u|^2} + D_T \frac{u_z^2}{|u|^2} \qquad (3.10)$$

$$D_{yy} = D_T \frac{u_x^2}{|u|^2} + D_L \frac{u_y^2}{|u|^2} + D_T \frac{u_z^2}{|u|^2} \qquad (3.11)$$

$$D_{zz} = D_T \frac{u_x^2}{|u|^2} + D_T \frac{u_y^2}{|u|^2} + D_L \frac{u_z^2}{|u|^2} \qquad (3.12)$$

$$D_{xy} = D_{yx} = (D_L - D_T) \frac{u_x . u_y}{|u|^2} \qquad (3.13)$$

$$D_{yz} = D_{zy} = (D_L - D_T) \frac{u_y . u_z}{|u|^2} \qquad (3.14)$$

$$D_{zx} = D_{xz} = (D_L - D_T) \frac{u_x . u_z}{|u|^2} \tag{3.15}$$

in which D_L and D_T are given by

$$D_L = \alpha_L \left|\frac{u}{n}\right| \tag{3.16}$$

$$D_T = \alpha_T \left|\frac{u}{n}\right| \tag{3.17}$$

where α_L = longitudinal dispersivity

α_T = transverse dispersivity

D_L = longitudinal dispersion coefficient (L^2T^{-1})

D_T = transverse dispersion coefficient (L^2T^{-1})

3.3. Finite Element Formulation:

3.3.1. One Dimensional Dispersion in One Dimensional Flow Field:

The basic differential equation describing the process of transport in saturated porous medium and accounting the effects of convection, hydrodynamic dispersion, adsorption, and radioactive decay can be expressed in Cartesian co-ordinate system

$$R \frac{\partial c}{\partial t} - D_{xx} \frac{\partial^2 c}{\partial x^2} + \frac{1}{n} \frac{\partial}{\partial x} (u_x c) + \lambda Rc - \frac{q}{n} c^* = 0 \tag{3.7}$$

Initial and boundary conditions are:

$$c(x, t) = 0 \quad \text{at} \quad t = 0 \text{ and } x \geq 0 \tag{3.18}$$

$$c(x, t) = c_o \quad \text{for} \quad t > 0 \text{ and } x = 0 \tag{3.19}$$

$$c(\infty, t) = 0 \quad \text{for} \quad t > 0 \tag{3.20}$$

Now we approximate the unknown concentration c and also the components of spatially dependent parameters in terms of basic functions $N_j(x, y)$ by

$$c \simeq c^{(e)}(x,\ t) = \sum_{j=1}^{n} N_j(x) \cdot \varphi_j(x) \tag{3.21}$$

$$= \lfloor N_1,\ N_2 \ldots \rfloor \begin{Bmatrix} \varphi_1(t) \\ \varphi_2(t) \\ \varphi_3(t) \\ \vdots \\ \varphi_n(t) \end{Bmatrix}$$

$$= \lfloor N_j \rfloor \{\varphi_j(t)\} \tag{3.22}$$

The approximating integral equations are obtained from Galerkin's scheme by making the residual, $\varepsilon^{(e)}$, generated by introducing (3.21) into (3.7) orthogonal to each of the N basis function N_j

$$\int N_i\ \varepsilon^{(e)}\ dx = 0 \tag{3.23}$$

$$\varepsilon^{(e)} = R\frac{\partial c^{(e)}}{\partial t} - D_{xx}\frac{\partial^2 c^{(e)}}{\partial x^2} + \frac{1}{n}\frac{\partial}{\partial x}(u_x c^{(e)}) + \lambda R c^{(e)} - \frac{q}{n} c^* \tag{3.24}$$

thus equation (3.23) becomes

$$\int_0^h N_i \left[R\frac{\partial c^{(e)}}{\partial t} - D_{xx}\frac{\partial^2 c^{(e)}}{\partial x^2} + \frac{1}{n}\frac{\partial}{\partial x}(u_x c^{(e)}) + \lambda R c^{(e)} - \frac{q}{n} c^* \right] dx = 0$$

i.e.

$$\int_0^h N_i\ R\frac{\partial c^{(e)}}{\partial t}\, dx - D_{xx}\int_0^h \frac{\partial^2 c^{(e)}}{\partial x^2}\, dx + \frac{1}{n}\int_0^h N_i \frac{\partial}{\partial x}(u_x c^{(e)})\, dx$$

$$+ \int_0^h N_i\ \lambda R c^{(e)}\, dx - \int_0^h N_i \frac{q}{n} c^*\, dx = 0$$

i.e.

$$\int_0^h N_i\, R \frac{\partial c^{(e)}}{\partial t}\, dx - D_{xx} N_i \frac{\partial c^{(e)}}{\partial x}\Big|_0^h + \int_0^h D_{xx} N_i' \frac{\partial c^{(e)}}{\partial x}\, dx$$

$$+ \frac{1}{n}\int_0^h N_i \frac{\partial}{\partial x}(u_x c^{(e)})\, dx + \int_0^h N_i\, \lambda R c^{(e)}\, dx - \int_0^h N_i \frac{q}{n} c^*\, dx = 0$$

i.e.

$$\int_0^h [R\, N_i N_j]\, dx \left\{\frac{\partial \varphi}{\partial t}\right\}^{ne} - D_{xx}\, N_i \frac{\partial c^{(e)}}{\partial x}\Big|_0^h + \left[D_{xx}\int_0^h (N_i' N_j')\, dx\right.$$

$$+ \frac{u_x}{n}\int_0^h (N_i N_j')\, dx + \lambda R \int_0^h \left[(N_i N_j)\, dx\right] \{\varphi\}^{ne} - \int_0^h N_i \frac{q}{n} c^*\, dx = 0 \tag{3.25}$$

writing equation (3.25) in matrix form

$$\int_0^h R\,\{N\}\lfloor N\rfloor\, dx\, \{\dot{\varphi}\}^{(ne)} + \left[D_{xx}\int_0^h \{N'\}\lfloor N'\rfloor\, dx\, +\right.$$

$$+ \frac{u_x}{n}\int_0^h \{N\}\lfloor N'\rfloor\, dx + \lambda R \int_0^h \{N\}\lfloor N\rfloor\, dx\quad \{\varphi\}^{(ne)}$$

$$= D_{xx}\, N_i \frac{\partial c}{\partial x}\Big|_0^h + \frac{q}{n} c^* \int_0^h \{N\}\, dx$$

$$[P]\left\{\frac{\partial \varphi}{\partial t}\right\}^{(ne)} + [K]^{(ne)}\{\varphi\}^{(ne)} = \{F\}^{(ne)} \tag{3.26}$$

where

$$[P] = \int_0^h R\,\{N\}\lfloor N\rfloor\, dx \tag{3.27}$$

$$[K] = D_{xx}\int_0^h \{N'\}\lfloor N'\rfloor\, dx + \frac{u_x}{n}\int_0^h \{N\}\lfloor N'\rfloor dx$$

$$+ \lambda R \int_0^h \{N\}\lfloor N\rfloor\, dx \tag{3.28}$$

$$\{F\} = D_{xx}\, N_i \frac{\partial c}{\partial x}\Big|_0^h + \frac{q}{n} c^* \int_0^h \{N\}\, dx \tag{3.29}$$

In order to solve this equation in time domain, an implicit finite difference scheme is used for approximating the time derivative as given below

$$\{\frac{\partial \varphi}{\partial t}\} = \frac{1}{\Delta t} (\{\varphi\}^{t+\Delta t} - \{\varphi\}^{t}) \qquad (3.30)$$

For better accuracy of results column vector $\{\varphi\}$, in the term $[K]\{\varphi\}$ on left hand side of equation (3.26), can be expressed as an average value at time steps t and $t+\Delta t$ i.e.

$$\{\varphi\} = \frac{1}{2} (\{\varphi\}^{t+\Delta t} + \{\varphi\}^{t}) \qquad (3.31)$$

Now from (3.26), (3.30) and (3.31)

$$(\frac{1}{\Delta t}[P] + \frac{1}{2}[K]) \{\varphi\}^{t+\Delta t} = (\frac{1}{\Delta t}[P] - \frac{1}{2}[K]) \{\varphi\}^{t} + \{F\} \qquad (3.32)$$

Equation (3.32) thus represents the general assembly of set of F.E.M. equations. Solution of equation (3.32) after proper incorporation of initial and boundary conditions, will yield the unknown values of concentrations at various nodal points.

According to Zienkiewicz (1979), equation (3.32) can be written as

$$(\frac{1}{\Delta t}[P] + \theta[K]) \{\varphi\}^{t+\Delta t} = (\frac{1}{\Delta t}[P] - (1-\theta) [K]) \{\varphi\}^{t} + \{F\} \qquad (3.33)$$

Equation (3.32) is the special case of equation (3.33) for $\theta = \frac{1}{2}$ (Crank-Nicholson case).

Case 1: To find elemental matrices for linear interpolation polynomials

Let the domain be subdivided into a number of parts called finite elements. Let a typical element have nodes J and K.

Assume the solution over the element as

$$c^{(e)} = a + bx \tag{3.34}$$

where a and b are functions of time.

At $x = 0$ (i.e. at node j), let $c^{(e)} = \varphi_1(t)$

At $x = h$ (i.e. at node k), let $c^{(e)} = \varphi_2(t)$

Then $\varphi_2 = \varphi_1 + bh \quad \therefore \quad b = \dfrac{\varphi_2 - \varphi_1}{h}$

Substituting the value of a and b in equation (3.34) and keeping in mind that φ_1 and φ_2 are the functions of time.

$$c^{(e)} = \varphi_1 + \frac{\varphi_2 - \varphi_1}{h} x = (1 - \frac{x}{h})\varphi_1 + \frac{x}{h}\varphi_2$$

$$= \lfloor (1 - \frac{x}{h}), \frac{x}{h} \rfloor \begin{Bmatrix} \varphi_1 \\ \varphi_2 \end{Bmatrix}$$

$$= \lfloor N(x) \rfloor \{\varphi(t)\}^{(ne)}$$

where $N(x) = \lfloor N_1(x), N_2(x) \rfloor$

$$\{\varphi(t)\}^{(ne)} = \begin{Bmatrix} \varphi_1(t) \\ \varphi_2(t) \end{Bmatrix}$$

$$N_1(x) = 1 - \frac{x}{h}$$

$$N_2(x) = \frac{x}{h}$$

For linear element compatibility of $c^{(e)}$ is needed and completeness of c and c' are also needed. In our element, compatibility

and completeness requirements are satisfied. Now

$$[P]^{(e)} = \int_0^h R\,\{N\}\lfloor N\rfloor\,dx = \frac{Rh}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

$$[K]^{(e)} = \int_0^h D_{xx}\{N'\}\lfloor N'\rfloor\,dx + \frac{u_x}{n}\int_0^h \{N\}\lfloor N'\rfloor dx$$

$$+ \lambda R\int_0^h \{N\}\lfloor N\rfloor dx$$

$$= \frac{D_{xx}}{h}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} + \frac{u_x}{2n}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \frac{\lambda Rh}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

$$\{F\}^{(ne)} = \{D_{xx} N_i \frac{\partial c^{(e)}}{\partial x}\Big|_0^h\} + \frac{q}{n} c^* \int_0^h \{N\}\,dx$$

$$= \begin{Bmatrix} D_{xx}(1 - \frac{x}{h})\,\frac{\partial c^{(e)}}{\partial x}\Big|_0^h \\ D_{xx}\cdot\frac{x}{h}\frac{\partial c^{(e)}}{\partial x}\Big|_0^h \end{Bmatrix} + \frac{q}{2n}\,c^* \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

$$= \begin{Bmatrix} -D_{xx}\frac{\partial c^{(e)}}{\partial x}\Big|_j \\ D_{xx}\frac{\partial c^{(e)}}{\partial x}\Big|_k \end{Bmatrix} + \frac{q}{2n}\,c^* \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

For one element equation (3.26) becomes

$$\frac{Rh}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}\begin{Bmatrix} \frac{\partial \varphi_1}{\partial t} \\ \frac{\partial \varphi_2}{\partial t} \end{Bmatrix} + (\frac{D_{xx}}{h}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} + \frac{u_x}{2n}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}$$

$$+ \frac{\lambda Rh}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{Bmatrix} \varphi_1 \\ \varphi_2 \end{Bmatrix} = \begin{Bmatrix} -D_{xx}\frac{\partial c^{(e)}}{\partial x}\Big|_1 \\ D_{xx}\frac{\partial c^{(e)}}{\partial x}\Big|_2 \end{Bmatrix} + \frac{q}{2n}\,c^*\begin{Bmatrix} 1 \\ 1 \end{Bmatrix} \tag{3.35}$$

For two elements,

$$\frac{Rh}{6}\begin{bmatrix} 2 & 1 & 0 \\ 1 & (2+2) & 1 \\ 0 & 1 & 2 \end{bmatrix}\begin{Bmatrix} \frac{\partial\varphi_1}{\partial t} \\ \frac{\partial\varphi_2}{\partial t} \\ \frac{\partial\varphi_3}{\partial t} \end{Bmatrix} + \Bigg(\frac{D_{xx}}{h}\begin{bmatrix} 1 & -1 & 0 \\ -1 & (1+1) & -1 \\ 0 & -1 & 1 \end{bmatrix}$$

$$+ \frac{u_x}{2n}\begin{bmatrix} -1 & 1 & 0 \\ -1 & 1-1 & 1 \\ 0 & 1 & 1 \end{bmatrix} + \frac{\lambda Rh}{6}\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2+2 & 1 \\ 0 & 1 & 2 \end{bmatrix}\Bigg)\begin{Bmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{Bmatrix}$$

$$\begin{Bmatrix} -D_{xx}\frac{\partial c^{(e)}}{\partial x}\Big|_1 \\ D_{xx}\frac{\partial c}{\partial x}\Big|_2 - D_{xx}\frac{\partial c_2}{\partial x}\Big|_2 \\ D_{xx}\frac{\partial c}{\partial x}\Big|_3 \end{Bmatrix} + \frac{q}{2n}c^{*}\begin{Bmatrix} 1 \\ 1+1 \\ 1 \end{Bmatrix}$$

i.e.

$$\frac{Rh}{6}\begin{bmatrix} 2 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 2 \end{bmatrix}\begin{Bmatrix} \frac{\partial\varphi_1}{\partial t} \\ \frac{\partial\varphi_2}{\partial t} \\ \frac{\partial\varphi_3}{\partial t} \end{Bmatrix} + \Bigg(\frac{D_{xx}}{h}\begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix} + \frac{u_x}{2n}\begin{bmatrix} -1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{bmatrix}$$

$$+ \frac{\lambda Rh}{6}\begin{bmatrix} 2 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 2 \end{bmatrix}\Bigg)\begin{Bmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{Bmatrix} = \begin{Bmatrix} -D_{xx}\frac{\partial c^{(e)}}{\partial x}\Big|_1 \\ 0 \\ D_{xx}\frac{\partial c^{(e)}}{\partial x}\Big|_2 \end{Bmatrix} + \frac{q}{2n}c^{*}h\begin{Bmatrix} 1 \\ 2 \\ 1 \end{Bmatrix}$$

(3.36)

For three elements

Assembled equation will be as follows:

$$\frac{Rh}{6}\begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 1 \\ 0 & 0 & 1 & 2 \end{bmatrix} \begin{Bmatrix} \frac{\partial \varphi_1}{\partial t} \\ \frac{\partial \varphi_2}{\partial t} \\ \frac{\partial \varphi_3}{\partial t} \\ \frac{\partial \varphi_4}{\partial t} \end{Bmatrix} + \left(\frac{D_{xx}}{h} \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix} \right.$$

$$\left. + \frac{u_x}{2n} \begin{bmatrix} -1 & 1 & 1 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 1 \end{bmatrix} + \frac{\lambda Rh}{6} \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 1 \\ 0 & 0 & 1 & 2 \end{bmatrix} \right) \begin{Bmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \varphi_4 \end{Bmatrix}$$

$$= \begin{Bmatrix} -D_{xx} \left.\frac{\partial c^{(e)}}{\partial x}\right|_1 \\ 0 \\ 0 \\ D_{xx} \left.\frac{\partial c^{(e)}}{\partial x}\right|_4 \end{Bmatrix} + \frac{q}{2n} c^* \begin{Bmatrix} 1 \\ 2 \\ 2 \\ 1 \end{Bmatrix} \qquad (3.37)$$

Initial and boundary conditions require to be incorporated at first node $\frac{\partial \varphi_1}{\partial t} = 0$ and $\left.\frac{\partial c^{(e)}}{\partial x}\right|_1$ = concentration gradient and $\varphi_1 = c_o$.

At last node $\frac{\partial \varphi_4}{\partial t} = 0$, and $\varphi_4 = 0$

Thus equation (3.37) becomes

$$\frac{Rh}{6}\begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 1 \\ 0 & 0 & 1 & 2 \end{bmatrix}\begin{Bmatrix} 0 \\ \frac{\partial\varphi_2}{\partial t} \\ \frac{\partial\varphi_3}{\partial t} \\ 0 \end{Bmatrix} + \left(\frac{D_{xx}}{h}\begin{bmatrix} +1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}\right.$$

$$\left. + \frac{u_x}{2n}\begin{bmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 1 \end{bmatrix} + \frac{\lambda Rh}{6}\begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 1 \\ 0 & 0 & 1 & 2 \end{bmatrix}\right)\begin{Bmatrix} c_o \\ \varphi_2 \\ \varphi_3 \\ 0 \end{Bmatrix} =$$

$$\begin{Bmatrix} -D_{xx}\left.\frac{\partial c^{(e)}}{\partial x}\right|_1 \\ 0 \\ 0 \\ D_{xx}\left.\frac{\partial c^{(e)}}{\partial x}\right|_4 \end{Bmatrix} + \frac{q}{2n}\ c^*\ h\begin{Bmatrix} 1 \\ 2 \\ 2 \\ 1 \end{Bmatrix} \qquad (3.38)$$

From equation (3.38) we will get two simultaneous equations in φ_2 and φ_3. We can solve for φ_2 and φ_3.

<u>Case 2</u>: Elemental matrices for quadratic elements

To find elemental matrices for quadratic elements, quadratic interpolation model for solution over element can be expressed as

$$c^{(e)}(x,\ t) = \alpha_1 + \alpha_2 x + \alpha_3 x^2 \qquad (3.39)$$

where α_1, α_2 and α_3 are the functions of time. Shape functions (N) are given in Appendix B.

$$[P]^{(e)} = R\int_o^h \{N\}\lfloor N\rfloor\, dx$$

$$[P]^{(e)} = \frac{Rh}{30}\begin{bmatrix} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{bmatrix}$$

Again

$$[K]^{(e)} = \int_0^h [D_{xx}\{N'\}\lfloor N'\rfloor + \frac{u_x}{n}\{N\}\lfloor N'\rfloor + \lambda R\{N\}\lfloor N\rfloor]dx$$

$$= \frac{D_{xx}}{3h}\begin{bmatrix} 7 & -8 & 1 \\ -8 & 16 & -8 \\ 1 & -8 & 7 \end{bmatrix} + \frac{u_x}{6n}\begin{bmatrix} -3 & 4 & -1 \\ -4 & 0 & 4 \\ 1 & -4 & 3 \end{bmatrix}$$

$$+ \frac{\lambda Rh}{30}\begin{bmatrix} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{bmatrix}$$

and

$$\{F\}^{ne} = \frac{q}{n} c^* \int_0^h \{N\}\, dx + \{D_{xx} N_i \frac{\partial c}{\partial n}\Big|_0^h\}$$

$$= \begin{Bmatrix} -D_{xx}\frac{\partial c}{\partial x}_1 \\ 0 \\ D_{xx}\frac{\partial c}{\partial x}_3 \end{Bmatrix} + \frac{q}{6n} c^* h \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix}$$

Thus for one element equation (3.26) can be written as

$$\frac{Rh}{30}\begin{bmatrix} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{bmatrix}\begin{Bmatrix} \frac{\partial \varphi_1}{\partial t} \\ \frac{\partial \varphi_2}{\partial t} \\ \frac{\partial \varphi_3}{\partial t} \end{Bmatrix} + (\frac{D_{xx}}{3h}\begin{bmatrix} 7 & -8 & 1 \\ -8 & 16 & -8 \\ 1 & -8 & 7 \end{bmatrix}$$

$$+ \frac{u_x}{6n} \begin{bmatrix} -3 & 4 & -1 \\ -4 & 0 & 4 \\ 1 & -4 & 3 \end{bmatrix} + \frac{\lambda Rh}{30} \begin{bmatrix} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{bmatrix}) \begin{Bmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{Bmatrix}$$

$$= \begin{Bmatrix} -D_{xx} \frac{\partial c}{\partial x}\Big|_1 \\ 0 \\ D_{xx} \frac{\partial c}{\partial x}\Big|_3 \end{Bmatrix} + \frac{q}{6n} c^* h \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix} \tag{3.40}$$

For two elements, the assembled equation becomes

$$\frac{Rh}{30} \begin{bmatrix} 4 & 2 & -1 & 0 & 0 \\ 2 & 16 & 2 & 0 & 0 \\ -1 & 2 & 8 & 2 & -1 \\ 0 & 0 & 2 & 16 & 2 \\ 0 & 0 & -1 & 2 & 4 \end{bmatrix} \begin{Bmatrix} \frac{\partial \varphi_1}{\partial t} \\ \frac{\partial \varphi_2}{\partial t} \\ \frac{\partial \varphi_3}{\partial t} \\ \frac{\partial \varphi_4}{\partial t} \\ \frac{\partial \varphi_5}{\partial t} \end{Bmatrix} + (\frac{D_{xx}}{3h} \begin{bmatrix} 7 & -8 & 1 & 0 & 0 \\ -8 & 16 & -8 & 0 & 0 \\ 1 & -8 & 14 & -8 & 1 \\ 0 & 0 & -8 & 16 & -8 \\ 0 & 0 & 1 & -8 & 7 \end{bmatrix}$$

$$+ \frac{u_x}{6n} \begin{bmatrix} -3 & 4 & -1 & 0 & 0 \\ -4 & 0 & 4 & 0 & 0 \\ 1 & -4 & 0 & 4 & -1 \\ 0 & 0 & -4 & 0 & 4 \\ 0 & 0 & 1 & -4 & -3 \end{bmatrix} + \frac{\lambda Rh}{30} \begin{bmatrix} 4 & 2 & -1 & 0 & 0 \\ 2 & 16 & 2 & 0 & 0 \\ -1 & 2 & 8 & 2 & -1 \\ 0 & 0 & 2 & 16 & 2 \\ 0 & 0 & -1 & 2 & 4 \end{bmatrix}) \begin{Bmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \varphi_4 \\ \varphi_5 \end{Bmatrix}$$

$$= \begin{Bmatrix} -D_{xx} \frac{\partial c}{\partial x}\Big|_1 \\ 0 \\ 0 \\ 0 \\ D_{xx} \frac{\partial c}{\partial x}\Big| \end{Bmatrix} + \frac{q}{6n} c^* h \begin{Bmatrix} 1 \\ 1 \\ 2 \\ 1 \\ 1 \end{Bmatrix} \tag{3.41}$$

Now at first node $\frac{\partial \varphi_1}{\partial t} = 0$ and $\left.\frac{\partial c^{(e)}}{\partial x}\right|_1$ = concentration gradient and $\varphi_1 = c_o$.

At last node $\frac{\partial \varphi_5}{\partial t} = 0$ and $\varphi_5 = 0$

Thus equation (3.41) becomes after incorporation of initial and boundary conditions

$$\begin{bmatrix} 4 & 2 & -1 & 0 & 0 \\ 2 & 16 & 2 & 0 & 0 \\ -1 & 2 & 8 & 2 & -1 \\ 0 & 0 & 2 & 16 & 2 \\ 0 & 0 & -1 & 2 & 4 \end{bmatrix} \begin{Bmatrix} 0 \\ \frac{\partial \varphi_2}{\partial t} \\ \frac{\partial \varphi_3}{\partial t} \\ \frac{\partial \varphi_4}{\partial t} \\ 0 \end{Bmatrix} + \left(\frac{D_{xx}}{3h} \begin{bmatrix} 7 & -8 & 1 & 0 & 0 \\ -8 & 16 & -8 & 0 & 0 \\ 1 & -8 & 14 & -8 & 1 \\ 0 & 0 & -8 & 16 & -8 \\ 0 & 0 & 1 & -8 & 7 \end{bmatrix}\right.$$

$$\left. + \frac{u_x}{6n} \begin{bmatrix} -3 & 4 & -1 & 0 & 0 \\ -4 & 0 & 4 & 0 & 0 \\ 1 & -4 & 0 & 4 & -1 \\ 0 & 0 & -4 & 0 & 4 \\ 0 & 0 & 1 & -4 & -3 \end{bmatrix} + \frac{\lambda R h}{30} \begin{bmatrix} 4 & 2 & -1 & 0 & 0 \\ 2 & 16 & 2 & 0 & 0 \\ -1 & 2 & 8 & 2 & -1 \\ 0 & 0 & 2 & 16 & 2 \\ 0 & 0 & -1 & 2 & 4 \end{bmatrix}\right) \begin{Bmatrix} c_o \\ \varphi_2 \\ \varphi_3 \\ \varphi_4 \\ 0 \end{Bmatrix}$$

$$\begin{Bmatrix} -D_{xx} \left.\frac{\partial c^{(e)}}{\partial x}\right|_1 \\ 0 \\ 0 \\ 0 \\ D_{xx} \left.\frac{\partial c^{(e)}}{\partial x}\right|_5 \end{Bmatrix} + \frac{q}{6n} c^* h \begin{Bmatrix} 1 \\ 1 \\ 2 \\ 1 \\ 1 \end{Bmatrix} \tag{3.42}$$

Equation (3.42) can be solved for φ_2, φ_3 and φ_4.

3.3.2. Two Dimensional Dispersion in Two Dimensional Flow Field:

Governing differential equation

$$R \frac{\partial c}{\partial t} - [D_{xx} \frac{\partial^2 c}{\partial x^2} + D_{xy} \frac{\partial^2 c}{\partial x \partial y} + D_{yx} \frac{\partial^2 c}{\partial y \partial x} + D_{yy} \frac{\partial^2 c}{\partial y^2}]$$

$$+ \frac{1}{n} [\frac{\partial}{\partial x} (u_x c) + \frac{\partial}{\partial y} (u_y c)] + \lambda R c - \frac{q}{n} c^* = 0 \qquad (3.8)$$

Initial and boundary conditions are:

$$c(x, y, t) = c_o \quad \text{for all } x, y \geq 0 \text{ and } t = 0 \qquad (3.43)$$

$$c(0, y, t) = c_o \quad \text{for } t > 0 \text{ and } 0 \leq y \leq \beta \qquad (3.44)$$

$$c(\infty, y, t) = 0 \quad \text{for } t > 0 \text{ and } 0 \leq y \leq \beta \qquad (3.45)$$

$$\frac{\partial c}{\partial y} (x, 0, t) = 0 \quad \text{for } t > 0 \qquad (3.46)$$

$$\frac{\partial c}{\partial y} (x, \beta, t) = \alpha \quad \text{for } t > 0 \text{ and } x > 0 \qquad (3.47)$$

Let the trial solution of equation (3.8) be assumed of the form

$$c(x, y, t) \simeq c^{(e)}(x, y, t) = \sum_{j=1}^{n} \lfloor N_j(x, y) \rfloor \{\varphi(t)\}^{(ne)}$$

$$= \lfloor N_1, N_2 \ldots N_n \rfloor \begin{Bmatrix} \varphi_1(t) \\ \varphi_2(t) \\ \vdots \\ \varphi_n(t) \end{Bmatrix} \qquad (3.48)$$

where $N_j(x, y)$ are the interpolation functions. $\varphi(t)$ are the unknown nodal values of concentrations.

The approximate function $c^{(e)}(x, y, t)$ will be exact solution to the equation (3.8) if the error or residual

$$\varepsilon^{(e)} = R\frac{\partial c^{(e)}}{\partial t} - [D_{xx}\frac{\partial^2 c^{(e)}}{\partial x^2} + D_{xy}\frac{\partial^2 c^{(e)}}{\partial y\,\partial x} + D_{yx}\frac{\partial^2 c^{(e)}}{\partial x\partial y} + D_{yy}\frac{\partial^2 c^{(e)}}{\partial y^2}$$

$$+ \frac{1}{n}[\frac{\partial}{\partial x}(u_x c^{(e)}) + \frac{\partial}{\partial y}(u_y c^{(e)})] + \lambda R c^{(e)} - \frac{q}{n} c^*$$

is equal to zero. (3.49)

To minimize the residual, applying Galerkin method,

$$\int\int_{A^{(e)}} N_i\, \varepsilon^{(e)}\, dA = 0$$

$$\int\int_{A^{(e)}} N_i\, [R\frac{\partial c^{(e)}}{\partial t} - (D_{xx}\frac{\partial^2 c^{(e)}}{\partial x^2} + D_{xy}\frac{\partial^2 c^{(e)}}{\partial x\,\partial y} + D_{yx}\frac{\partial^2 c^{(e)}}{\partial y\partial x} + D_{yy}\frac{\partial^2 c^{(e)}}{\partial y^2})$$

$$+ \frac{1}{n}[\frac{\partial}{\partial x}(u_x c^{(e)}) + \frac{\partial}{\partial y}(u_y c^{(e)})] + \lambda R c^{(e)} - \frac{q}{n} c^*]\, dx\, dy = 0 \quad (3.50)$$

$$\int\int_{A^{(e)}} D_{xx} N_i \frac{\partial^2 c^{(e)}}{\partial x^2}\, dx\, dy = \oint D_{xx} N_i \frac{\partial c}{\partial x} l_x\, ds - \int\int_{A^{(e)}} D_{xx}\frac{\partial N_i}{\partial x}\frac{\partial c^{(e)}}{\partial x}\, dx\, dy$$

$$= \oint D_{xx} N_i \frac{\partial c}{\partial x} l_x\, ds - \int\int_{A^{(e)}} D_{xx}\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}\, dA\, \{\varphi\}^{(ne)}$$

$$\int\int_{A^{(e)}} N_i\, D_{yy}\frac{\partial^2 c^{(e)}}{\partial y^2}\, dx\, dy = \oint D_{yy} N_i \frac{\partial c}{\partial y} l_y\, ds$$

$$- \int\int_{A^{(e)}} D_{yy}\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}\, dA\, \{\varphi\}^{(ne)}$$

$$\int\int_{A^{(e)}} D_{xy} N_i \frac{\partial^2 c}{\partial x\partial y}\, dx\, dy = \oint D_{xy} N_i \frac{\partial c}{\partial y} l_x\, ds$$

$$- \int\int_{A^{(e)}} D_{xy}\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial y}\, dA\, \{\varphi\}^{(ne)}$$

$$\int\int_{A^{(e)}} D_{yx} N_i \frac{\partial^2 c}{\partial y\partial x}\, dx\, dy = \oint D_{yx} N_i \frac{\partial c}{\partial x} l_y\, ds$$

$$- \int\int_{A^{(e)}} D_{yx}\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial x}\, dA\, \{\varphi\}^{(ne)}$$

$$\int\int_{A^{(e)}} \frac{u_x}{n} N_i \frac{\partial c}{\partial x} dx\, dy = \oint \frac{u_x}{n} N_i\, c\, l_x\, ds - \int\int_{A^{(e)}} \frac{u_x}{n} \frac{\partial N_i}{\partial x} N_j\, dA\, \{\varphi\}^{(ne)}$$

$$\int\int_{A^{(e)}} \frac{u_y}{n} N_i \frac{\partial c}{\partial y} dx\, dy = \oint \frac{u_y}{n} N_i\, c\, l_y\, ds - \int\int_{A^{(e)}} \frac{u_y}{n} \frac{\partial N_i}{\partial y} N_j\, dA\, \{\varphi\}^{(ne)}$$

Now equation (3.50) can be written as

$$\int\int_{A^{(e)}} [RN_iN_j]\, dA\, \{\frac{\partial \varphi}{\partial t}\}^{(ne)} + \int\int_{A^{(e)}} [D_{xx} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + D_{xy} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y}$$

$$+ D_{yx} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} + D_{yy} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} - \frac{u_x}{n} \frac{\partial N_i}{\partial x} N_j$$

$$- \frac{u_y}{n} \frac{\partial N_i}{\partial y} N_j + \lambda R\, N_iN_j]\, dA\, \{\varphi\}^{(ne)}$$

$$= \oint [(D_{xx} \frac{\partial c}{\partial x} + D_{xy} \frac{\partial c}{\partial y} - \frac{u_x}{n} c)\, l_x + (D_{yx} \frac{\partial c}{\partial x} + D_{yy} \frac{\partial c}{\partial y} - \frac{u_y}{n} c) l_y]\, N_i\, ds$$

$$+ \int\int_{A^{(e)}} \frac{q}{n} c^* \{N_i\} dA \qquad (3.51)$$

Writing equation (3.51) in matrix form

$$\int\int_{A^{(e)}} R\, \{N\}\lfloor N \rfloor\, dA\, \{\dot{\varphi}\}^{(ne)} + \int\int_{A^{(e)}} (D_{xx} \{N,_x\}\lfloor N,_x \rfloor + D_{xy} \{N,_x\}\lfloor N,_y \rfloor$$

$$+ D_{yx} \{N,_y\}\lfloor N,_x \rfloor + D_{yy} \{N,_y\}\lfloor N,_y \rfloor - \frac{u_x}{n} \{N,_x\}\lfloor N \rfloor - \frac{u_y}{n} \{N,_y\}\lfloor N \rfloor$$

$$+ \lambda R\, \{N\}\lfloor N \rfloor)\, dA\, \{\varphi\}^{(ne)}$$

$$= \oint [(D_{xx} \frac{\partial c}{\partial x} + D_{xy} \frac{\partial c}{\partial y} - \frac{u_x}{n} c) l_x + (D_{yx} \frac{\partial c}{\partial x} + D_{yy} \frac{\partial c}{\partial y} - \frac{u_y}{n} c) l_y]\, N_i\, ds$$

$$+ \int\int_{A^{(e)}} \frac{q}{n} c^* \{N\}\, dA \qquad (3.52)$$

Equation (3.52) can be written as

$$[P]\ \{\dot{\varphi}\}^{(ne)} + [K]\ \{\varphi\}^{(ne)} = \{F_B\} + \{F\} \tag{3.53}$$

where

$$[P] = \iint_{A^{(e)}} R\ \{N\}\lfloor N \rfloor\ dA$$

$$[K] = \iint_{A^{(e)}} (D_{xx}\ \{N,_x\}\lfloor N,_x\rfloor + D_{xy}\ \{N,_x\}\lfloor N,_y\rfloor + D_{yx}\ \{N,_y\}\lfloor N,_x\rfloor$$

$$+ D_{yy}\ \{N,_y\}\lfloor N,_y\rfloor - \frac{u_x}{n}\ \{N,_x\}\lfloor N\rfloor - \frac{u_y}{n}\ \{N,_y\}\lfloor N\rfloor$$

$$+ \lambda R\ \{N\}[N])\ dA$$

$$\{F_B\} = \oint [(D_{xx}\frac{\partial c}{\partial x} + D_{xy}\frac{\partial c}{\partial y} - \frac{u_x}{n}\ c)\,l_x$$

$$+ (D_{yx}\frac{\partial c}{\partial x} + D_{yy}\frac{\partial c}{\partial y} - \frac{u_y}{n})\,l_y\,]\,N_i\ ds$$

$$\{F\} = \iint_{A^{(e)}} \frac{q}{n}\ c^*\ \{N\}\ dA$$

In order to solve the equation in time domain, an implicit finite difference scheme is used for approximating the time derivative as given below

$$\{\dot{\varphi}\}^{(ne)} = \frac{\{\varphi\}^{t+\Delta t} - \{\varphi\}^{t}}{\Delta t}$$

For better accuracy of results, the column vector $\{\varphi\}^{(ne)}$ in term $[K]\ \{\varphi\}^{(ne)}$ on left hand side of equation (3.53) can be expressed as an average values at time t and (t + t), i.e.

$$\{\varphi\}^{(ne)} = \frac{1}{2}\,(\{\varphi\}^{t+\Delta t} + \{\varphi\}^{t})$$

Substituting the values of $\{\dot{\varphi}\}^{(ne)}$ and $\{\varphi\}^{(ne)}$ in equation (3.53)

$$(\frac{1}{\Delta t}[P] + \frac{1}{2}[K])\{\varphi\}^{t+\Delta t} = (\frac{1}{\Delta t}[P] - \frac{1}{2}[K])\{\varphi\}^{t} + \{F\} + \{F_B\} \tag{3.54}$$

Equation (3.54) thus represents the general assembly of set of F.E.M. equations, solution of equation (3.54) after proper incorporation of initial and boundary conditions, will yield the unknown values of concentrations at various nodal points.

Now according to Zienkiewicz (1979), equation (3.54) can be written as

$$(\frac{1}{\Delta t}[P] + \theta[K])\{\varphi\}^{t+\Delta t} = (\frac{1}{\Delta t}[P] - (1-\theta)[K])\{\varphi\}^{t} + \{F_B\} + \{F\} \tag{3.55}$$

Equation (3.55) is the special case for $\theta = \frac{1}{2}$ (Crank-Nicholson case). In order to solve the equation we need compatibility of c and completeness of c, $\frac{\partial c}{\partial x}$ and $\frac{\partial c}{\partial y}$. For this assume a suitable form of variation of concentration $c^{(e)}$ inside a finite element 'e'. We assume a linear variation as

$$c^{(e)}(x, y, t) = \alpha_1 + \alpha_2 x + \alpha_3 y \tag{3.56}$$

where α_1, α_2 and α_3 are the functions of time.

<u>Calculation of Elemental Matrices</u>: Shape functions (N) for triangular elements are given in Appendix B. Now

$$\frac{\partial N_1}{\partial x} = \frac{b_1}{2A^{(e)}}, \quad \frac{\partial N_2}{\partial x} = \frac{b_2}{2A^{(e)}}, \quad \frac{\partial N_3}{\partial x} = \frac{b_3}{2A^{(e)}}, \quad \frac{\partial N_1}{\partial y} = \frac{c_1}{2A^{(e)}},$$

$$\frac{\partial N_2}{\partial y} = \frac{c_2}{2A^{(e)}}, \quad \frac{\partial N_3}{\partial y} = \frac{c_3}{2A^{(e)}}$$

Now

$$[P] = \int\int_{A^{(e)}} R\,\{N\}\lfloor N \rfloor\, dA$$

$$= \int\int_{A^{(e)}} R \begin{Bmatrix} N_1 \\ N_2 \\ N_3 \end{Bmatrix} \lfloor N_1 \quad N_2 \quad N_3 \rfloor\, dA$$

$$= R \int\int_{A^{(e)}} \begin{bmatrix} N_1^2 & N_1N_2 & N_1N_3 \\ N_2N_1 & N_2^2 & N_2N_3 \\ N_3N_1 & N_3N_2 & N_3^2 \end{bmatrix} dA$$

$$= \frac{RA^{(e)}}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

$$\int\int_{A^{(e)}} D_{xx}\,\{N,_x\}\lfloor N,_x \rfloor\, dA = D_{xx} \int\int_{A^{(e)}} \begin{Bmatrix} \frac{\partial N_1}{\partial x} \\ \frac{\partial N_2}{\partial x} \\ \frac{\partial N_3}{\partial x} \end{Bmatrix} \lfloor \frac{\partial N_1}{\partial x} \quad \frac{\partial N_2}{\partial x} \quad \frac{\partial N_3}{\partial x} \rfloor\, dA$$

$$= D_{xx} \int\int_{A^{(e)}} \begin{Bmatrix} \frac{b_1}{2A^{(e)}} \\ \frac{b_2}{2A^{(e)}} \\ \frac{b_3}{2A^{(e)}} \end{Bmatrix} \frac{1}{2A^{e}} \lfloor b_1 \quad b_2 \quad b_3 \rfloor\, dA$$

$$= \frac{D_{xx}}{4A^{(e)}} \begin{bmatrix} b_1^2 & b_1b_2 & b_1b_3 \\ b_2b_1 & b_2^2 & b_2b_3 \\ b_3b_1 & b_3b_2 & b_3^2 \end{bmatrix}$$

$$\int\int_{A^{(e)}} D_{xy}\ \{N,_x\}\lfloor N,_y\rfloor\ dA = \frac{D_{xy}}{4A^{(e)}} \begin{bmatrix} b_1c_1 & b_1c_2 & b_1c_3 \\ b_2c_1 & b_2c_2 & b_2c_3 \\ b_3c_1 & b_3c_2 & b_3c_3 \end{bmatrix}$$

$$\int\int_{A^{(e)}} D_{yx}\ \{N,_y\}\lfloor N,_x\rfloor\ dA = \frac{D_{yx}}{4A^{(e)}} \begin{bmatrix} c_1b_1 & c_1b_2 & c_1b_3 \\ c_2b_1 & c_2b_2 & c_2b_3 \\ c_3b_1 & c_3b_2 & c_3b_3 \end{bmatrix}$$

$$\int\int_{A^{(e)}} D_{yy}\ \{N,_y\}\lfloor N,_y\rfloor\ dA = \frac{D_{yy}}{4A^{(e)}} \begin{bmatrix} c_1^2 & c_1c_2 & c_1c_3 \\ c_2c_1 & c_2^2 & c_2c_3 \\ c_3c_1 & c_3c_2 & c_3^2 \end{bmatrix}$$

$$\int\int_{A^{(e)}} \frac{u_x}{n}\ \{N,_x\}[N]\ dA = \int\int_{A^{(e)}} \frac{u_x}{n} \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \end{Bmatrix} \lfloor N_1 \quad N_2 \quad N_3\rfloor\ dA$$

$$= \frac{u_x}{2nA^{(e)}} \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \end{Bmatrix} \left\lfloor \frac{A^{(e)}}{3} \quad \frac{A^{(e)}}{3} \quad \frac{A^{(e)}}{3} \right\rfloor$$

$$= \frac{u_x}{6n} \begin{bmatrix} b_1 & b_1 & b_1 \\ b_2 & b_2 & b_2 \\ b_3 & b_3 & b_3 \end{bmatrix}$$

$$\int\int_{A^{(e)}} \frac{u_y}{n}\ \{N,_y\}\lfloor N\rfloor\ dA = \frac{u_y}{6n} \begin{bmatrix} c_1 & c_1 & c_1 \\ c_2 & c_2 & c_2 \\ c_3 & c_3 & c_3 \end{bmatrix}$$

$$\int\int_{A^{(e)}} \lambda R\ \{N\}\lfloor N_j\rfloor\ dA = \frac{\lambda R A^{(e)}}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

Thus

$$[K] = \frac{D_{xx}}{4A^{(e)}} \begin{bmatrix} b_1^2 & b_1b_2 & b_1b_3 \\ b_2b_1 & b_2^2 & b_2b_3 \\ b_3b_1 & b_3b_2 & b_3^2 \end{bmatrix} + \frac{D_{xy}}{4A^{(e)}} \cdot \begin{bmatrix} b_1c_1 & b_1c_2 & b_1c_3 \\ b_2c_1 & b_2c_2 & b_2c_3 \\ b_3c_1 & b_3c_2 & b_3c_3 \end{bmatrix}$$

$$+ \frac{D_{yx}}{4A^{(e)}} \begin{bmatrix} c_1b_1 & c_1b_2 & c_1b_3 \\ c_2b_1 & c_2b_2 & c_2b_3 \\ c_3b_1 & c_3b_2 & c_3b_3 \end{bmatrix} + \frac{D_{yy}}{4A^{(e)}} \begin{bmatrix} c_1^2 & c_1c_2 & c_1c_3 \\ c_2c_1 & c_2^2 & c_2c_3 \\ c_3c_1 & c_3c_2 & c_3^2 \end{bmatrix}$$

$$- \frac{u_x}{6n} \begin{bmatrix} b_1 & b_1 & b_1 \\ b_2 & b_2 & b_2 \\ b_3 & b_3 & b_3 \end{bmatrix} - \frac{u_y}{6n} \begin{bmatrix} c_1 & c_1 & c_1 \\ c_2 & c_2 & c_2 \\ c_3 & c_3 & c_3 \end{bmatrix}$$

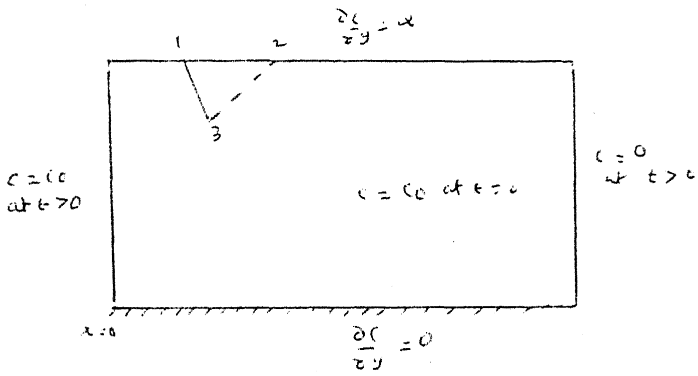
$$+ \frac{\lambda R A^{(e)}}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

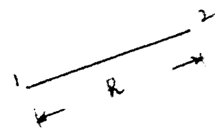
$$\{F\} = \iint_{A^{(e)}} \frac{q}{n} c^* \{N\}\, dA = \frac{q}{3n} c^* A^{(e)} \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix}$$

<u>To Calculate Contour Integral</u>:

$$F_B = \oint \Big[\Big(D_{xx} \frac{\partial c}{\partial x} + D_{xy} \frac{\partial c}{\partial y} - \frac{u_x}{n} c\Big) l_x + \Big(D_{yx} \frac{\partial c}{\partial x} + D_{yy} \frac{\partial c}{\partial y} - \frac{u_y}{n} c\Big) l_y \Big] N_i \, ds$$

on boundary where $\frac{\partial c}{\partial y} = \alpha$





$$F_B = \oint [(D_{xx} \frac{\partial c}{\partial x} + \alpha\, D_{xy} - \frac{u_x}{n} c) l_x$$

$$+ (D_{yx} \frac{\partial c}{\partial x} + \alpha\, D_{xy} - \frac{u_y}{n}) l_y]\, N_i \, ds$$

Let the 1-2 is boundary of an element triangle 1 2 3.

Let distribution on 1-2 is

$$c = N_1 \varphi_1 + N_2 \varphi_2$$

$$N_1 = 1 - \frac{s}{h} \Rightarrow \frac{N_1}{s} = -\frac{1}{h} \qquad \frac{dy}{dx} = \tan\theta, \quad \frac{dy}{ds} = \sin\theta$$

$$N_2 = \frac{s}{h} \Rightarrow \frac{N_2}{s} = \frac{1}{h} \qquad \frac{dx}{ds} = \cos\theta$$

$$\frac{\partial c}{\partial x} = \frac{\partial N_1}{\partial x} \varphi_1 + \frac{\partial N_2}{\partial x} \varphi_2 = \frac{\partial N_1}{\partial s} \frac{\partial s}{\partial x} \varphi_1 + \frac{\partial N_2}{\partial s} \frac{\partial s}{\partial x} \varphi_2$$

$$= -\frac{1}{h\cos\theta} \varphi_1 + \frac{1}{h\cos\theta} \varphi_2 = \frac{1}{h\cos\theta} [\varphi_2 - \varphi_1]$$

$$\frac{\partial c}{\partial y} = \frac{\partial N_1}{\partial y} \varphi_1 + \frac{\partial N_2}{\partial y} \varphi_2 = \frac{\partial N_1}{\partial s} \frac{\partial s}{\partial y} \varphi_1 + \frac{\partial N_2}{\partial s} \frac{\partial s}{\partial y} \varphi_2 = \frac{1}{h\sin\theta} [\varphi_2 - \varphi_1]$$

$$\oint D_{xx} \frac{\partial c}{\partial x} N_i \, ds = \int_0^h D_{xx} \frac{1}{h\cos\theta} (\varphi_2 - \varphi_1) \begin{Bmatrix} 1 - \frac{s}{h} \\ \frac{s}{h} \end{Bmatrix} l_x \, ds$$

$$= \int_0^h D_{xx} \frac{1}{h\cos\theta}(\varphi_2-\varphi_1) \begin{Bmatrix} 1-\frac{s}{h} \\ \frac{s}{h} \end{Bmatrix} \cos\theta \, ds = \frac{D_{xx}}{h}(\varphi_2-\varphi_1) \begin{Bmatrix} h/2 \\ h/2 \end{Bmatrix}$$

$$= \frac{D_{xx}}{2}(\varphi_2-\varphi_1) \begin{Bmatrix} 1 \\ 1 \end{Bmatrix} = \frac{D_{xx}}{2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \begin{Bmatrix} \varphi_1 \\ \varphi_2 \end{Bmatrix}$$

$$\oint D_{xy}\, \alpha\, N_i\, l_x\, ds = \int_0^h D_{xy}\, \alpha \cos\theta \begin{Bmatrix} 1-\frac{s}{h} \\ \frac{s}{h} \end{Bmatrix} ds$$

$$= \frac{D_{xy}}{2} \alpha\, h\cos\theta \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

$$\oint D_{yx} \frac{\partial c}{\partial x} l_y\, N_i\, ds = \int_0^h D_{yx} \frac{1}{h\cos\theta}(\varphi_2-\varphi_1) \begin{Bmatrix} 1-\frac{s}{h} \\ \frac{s}{h} \end{Bmatrix} \sin\theta \, ds$$

$$= \tan\theta \frac{D_{yx}}{h}(\varphi_2-\varphi_1) \begin{Bmatrix} h/2 \\ h/2 \end{Bmatrix}$$

$$= \frac{D_{yx}}{2} \tan\theta \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \begin{Bmatrix} \varphi_1 \\ \varphi_2 \end{Bmatrix}$$

$$\oint D_{yy} \frac{\partial c}{\partial y} l_y\, N_i\, ds = \int_0^h D_{yy}\, \alpha \sin\theta \begin{Bmatrix} 1-\frac{s}{h} \\ \frac{s}{h} \end{Bmatrix} ds = \frac{D_{yy}}{2} \alpha \sin\theta\, h \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

$$\oint \frac{u_x}{n} c\, N_i\, l_x\, ds = \int_0^h \frac{u_x}{n} \lfloor N_1\varphi_1 + N_2\varphi_2 \rfloor \begin{Bmatrix} N_1 \\ N_2 \end{Bmatrix} \cos\theta\, ds$$

$$= \frac{u_x\, h\cos\theta}{6n} \begin{Bmatrix} 2\varphi_1 + \varphi_2 \\ \varphi_1 + 2\varphi_2 \end{Bmatrix}$$

$$= \frac{h\, u_x \cos\theta}{6n} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{Bmatrix} \varphi_1 \\ \varphi_2 \end{Bmatrix}$$

Similarly

$$\oint \frac{u_y}{n} c \ N_i \ l_y \ ds = \frac{h \ u_y \sin\theta}{6n} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{Bmatrix} \varphi_1 \\ \varphi_2 \end{Bmatrix}$$

$$[F_B]_1^2 = \oint [(D_{xx} \frac{\partial c}{\partial x} + D_{xy} \alpha - \frac{u_x}{n} c) l_x$$

$$+ (D_{yx} \frac{\partial c}{\partial x} + D_{yy} \alpha - \frac{u_y}{n} c) l_y] N_i \ ds$$

$$= (\frac{D_{xx}}{2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \frac{D_{yx}}{2} \tan\theta \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \frac{h \ u_x \cos\theta}{6n} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

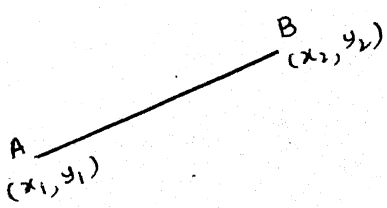
$$+ \frac{h \ u_y \sin\theta}{6n} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}) \begin{Bmatrix} \varphi_1 \\ \varphi_2 \end{Bmatrix}$$

$$+ \frac{D_{xy}}{2} \alpha \ h \cos\theta \begin{Bmatrix} 1 \\ 1 \end{Bmatrix} + \frac{D_{yy}}{2} \alpha \ h \sin\theta \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

$$= [(\frac{D_{xx}}{2} + \frac{D_{yx}}{2} \tan\theta) \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} +$$

$$\frac{h}{6n} (u_x \cos\theta + u_y \sin\theta) \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}] \begin{Bmatrix} \varphi_1 \\ \varphi_2 \end{Bmatrix}$$

$$+ \frac{1}{2} h \ \alpha \ (D_{xy} \cos\theta + D_{yy} \sin\theta) \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$



$$h = ((x_2 - x_1)^2 + (y_2 - y_1)^2)^{1/2}$$

$$= (b_3^2 + c_3^2)^{1/2}$$

$$\tan\theta = \frac{y_2 - y_1}{x_2 - x_1} = - \frac{b_3}{c_3}$$

$$\sin\theta = - \frac{b_3}{(b_3^2 + c_3^2)^{1/2}} = - \frac{b_3}{h}$$

$$\cos\theta = \frac{c_3}{(b_3^2 + c_3^2)^{1/2}} = \frac{c_3}{h}$$

$$[F_B]_1^2 = [\tfrac{1}{2}(D_{xx} - D_{yx}\frac{b_3}{c_3}) \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \frac{1}{6n}(u_x c_3 - u_y b_3) \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}] \begin{Bmatrix} \varphi_1 \\ \varphi_2 \end{Bmatrix}$$

$$+ \frac{\alpha}{2}(D_{xy}\ c_3 - D_{xy}\ b_3) \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

Similarly when 2-3 are the boundary nodes

$$[F_B]_2^3 = [(\frac{D_{xx}}{2} - \frac{D_{yx}}{2}\frac{b_1}{c_1}) \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \frac{1}{6n}(u_x c_1 - u_y b_1) \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}] \begin{Bmatrix} \varphi_2 \\ \varphi_3 \end{Bmatrix}$$

$$+ \frac{\alpha}{2}(D_{xy}\ c_1 - D_{yy}\ b_1) \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

When 3-1 are the boundary nodes

$$[F_B]_3^1 = [\tfrac{1}{2}(D_{xx} - D_{yx}\frac{b_2}{c_2}) \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \frac{1}{6n}(u_x c_2 - u_y b_2) \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}] \begin{Bmatrix} \varphi_3 \\ \varphi_1 \end{Bmatrix}$$

$$+ \frac{\alpha}{2}[D_{xy}\ c_2 - D_{yy}\ b_2] \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

Equation (3.8) is also solved on the same lines as above for second set of initial and boundary conditions which are given below:

$$c(x, y, t) = c_o \quad \text{for all } x, y \geq 0 \text{ at } t = 0 \qquad (3.43)$$

$$c(0, y, t) = 0 \quad \text{for } t > 0 \text{ and } 0 \leq y \leq \beta \qquad (3.57)$$

$$c(\ , y, t) = 0 \quad \text{for } t > 0 \text{ and } 0 \leq y \leq \beta \qquad (3.45)$$

$$\frac{\partial c}{\partial y}(x, 0, t) = 0 \quad \text{for } t > 0 \qquad (3.44)$$

$$c(x, \beta, t) = 0 \quad \text{for } t > 0 \qquad (3.58)$$

CHAPTER 4

RESULTS AND DISCUSSION

4.1. General:

In the present work one dimensional and two dimensional dispersion equations for predicting the pollutant concentration in groundwater flow have been solved using the finite element technique. In the one dimensional case both linear and quadratic elements have been considered. In two dimensional case triangular elements have been taken and the equation has been solved for two different sets of boundary conditions. In solving a dispersion equation a suitable value of θ has to be choosen. To find the optimum θ, the one dimensional equation was solved for different values of θ and time intervals. It was noticed that at the value of $\theta = 0.75$ the analytical results matched closely with the results obtained by the finite element method. The concentration values for different values of θ for $t = 15$ min, are shown in Table 2. Based on these results θ is choosen to be 0.75 for all subsequent calculations. The various results for both one dimensional and two dimensional cases have been discussed in the following paragraphs.

4.2. One Dimensional Case:

In one dimensional case dispersion equation was solved by taking both linear and quadratic elements and results obtained are compared with the analytical results.

4.2.1. Linear Elements:

Case 1: The dispersion equation was solved for the special case where the retardation R is taken equal to 1. Volumetric fluid injection rate q and concentration of source fluid c^* are respectively zero velocity in x direction is taken as 0.039 m/min and porosity as 0.39. The equation was solved by using both analytical and F.E.M. methods for different time intervals. The results have been presented in Figure 4.1. It is seen that the results obtained by the two methods match closely with deviation never being more than 3 percent. Slight deviation in the finite element results might be due to the following reasons: firstly inaccuracy may result due to semi-implicit-explicit finite difference scheme used for approximating the time derivative. Secondly, due to comparatively larger value of time interval used. Thirdly, due to the effect of finite boundary which was taken as 50 m in this case, lastly, due to the length of element choosen.

Case 2: The same equation was solved by changing the value of R from 1 to 1.156. The corresponding results are shown in Figure 4.2.

Case 3: In this case the value of λ (for radium) is changed from 0 to 4.343×10^{-8} per min. The results are found to be the same as for Case 2. Thus it may be concluded that when the value of λ is less it does not have significant effect on the concentration distribution.

Case 4: In this case the value of q is changed to 0.006 per min and c^* to 10 mg/L and all other values are same as in first case. The results are shown in Figure 4.3. At some distance from the source, the concentration is more than initial concentration. This is due to volumetric fluid injection rate and concentration of source fluid. It is seen that after some distance concentration stabilises.

Case 5: In this case, the value of R (retardation factor) is changed from 1 to 1.156 and all other values are kept same as in previous case. The results are shown in Figure 4.4. It is seen that the nature of variation is same as in Figure 4.3, though because of adsorption pollutant concentrations are less in this case.

Case 6: In this case all values are kept same as in first one. Only the value of λ was taken as 4.34×10^{-8} per min. This variation is shown in Figure 4.5.

Quadratic case: The dispersion equation was solved for all the cases described in previous sections using quadratic elements. The results match closely with those obtained for linear cases (Figures 4.1 to 4.5).

Comparison of results when the problem was solved by linear approximation (Figure 4.1) and quadratic approximation (Figure 4.6) for the same set of values show that the results closely match each other. It is also seen that the results obtained by quadratic method match even more closely with the analytical results than those obtained by linear method.

4.3. Two Dimensional Case:

Two dimensional dispersion equation is solved using finite element method by using triangular elements. The governing equation was solved for two different sets of boundary conditions described below. Results for one set of boundary conditions are given in Figures 4.7a and 4.7b.

The domain was taken as rectangular area 100 m in x direction and 30 m in y direction. This area is divided into square elements 5 m x 5 m which are again divided into triangular elements thus giving 240 elements with 147 nodes. Initial concentration of pollutant is taken as 5.0 mg/L all over the domain. In this case the value of retardation factor (R) is taken as 1.0, D_{xx} and D_{yy} are taken as 6×10^{-5} m^2/min and 9×10^{-6} m^2/min respectively, the velocities in x direction and y direction (u_x and u_y) are taken as 0.06 m/min and 0.012 m/min respectively. Value of α is 0.1 mg/L per meter and the values of cross coefficients of dispersion D_{xy}, D_{yx} and λ, q and c are all zero.

The dispersion equation is solved for the first set of boundary conditions shown in Figure 4.8 The concentration at different time intervals are found at all the nodes in the domain. From this, contour of concentration of pollutants at various time intervals are plotted.

Figure 4.7(a) shows the results for t = 10 min and Figure 4.7(b) for t = 25 min. From Figures 4.7(a) and 4.7(b) it is seen that near impervious boundary concentration gradient is high. Near the boundary at which the concentration is specified as

5.0 mg/L, the concentration gradient is also high. As we go away from the impervious boundary as well as specified boundaries the concentration is almost same (i.e. concentration gradient is very small) and it decreases with time.

TABLE 2. COMPARISON OF RESULTS FOR LINEAR ELEMENTS AFTER 5 MINUTES

Distance x in m	Exact solution	$\theta = 0.0$			$\theta = 0.5$			$\theta = 2.3$			
		$\Delta t =$ 0.5	$\Delta t =$ 1.0	$\Delta t =$ 2.5	$\Delta t =$ 0.5	$\Delta t =$ 1.0	$\Delta t =$ 2.5	$\Delta t =$ 0.5	$\Delta t =$ 1.0	$\Delta t =$ 2.5	$\Delta t =$ 5.0
0.00	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
1.0	4.9013	6.358	-119.5	76.91	5.174	5.187	5.83	4.1148	5.069	5.081	4.45
2.0	1.1267	3.200	-150.52	14.71	1.291	1.276	1.079	1.2987	1.294	1.238	1.188
3.0	0.1088	2.341	-84.37	1.717	0.1086	0.105	0.137	0.1366	0.1616	0.2308	0.3174

Distance x in m	Exact solution	$\theta = 0.75$				$\theta = 0.875$				$\theta = 1.0$			
		$\Delta t =$ 0.5	$\Delta t =$ 1.0	$\Delta t =$ 2.5	$\Delta t =$ 5.0	$\Delta t =$ 0.5	$\Delta t =$ 1.0	$\Delta t =$ 2.5	$\Delta t =$ 5.0	$\Delta t =$ 0.5	$\Delta t =$ 1.0	$\Delta t =$ 2.5	$\Delta t =$ 5.0
0.00	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
1.0	4.9013	5.085	5.009	4.856	4.314	5.04	4.92	4.606	6.624	4.995	4.583	4.416	3.91
2.0	1.1267	1.3027	1.20	1.216	1.289	1.309	1.321	1.347	3.837	1.3166	1.338	1.341	1.429
3.0	0.1088	0.141	0.115	0.273	0.375	0.1684	0.218	0.331	2.222	0.186	0.0958	0.383	0.522

contd...

Table 2 (continued). COMPARISON OF RESULTS FOR LINEAR ELEMENTS AFTER 10 MINUTES

Distance x in m	Exact solution	$\theta = 0.0$		$\theta = 0.5$		$\theta = 2/3$			$\theta = 0.75$		
		$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$
0.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
1.0	7.138	36676.6	3999.8	7.247	7.4515	7.182	7.1245	7.291	7.148	7.0323	6.976
2.0	3.649	62831.8	3151.2	3.8225	3.8641	8.7672	3.695	3.498	3.67	3.632	3.431
3.0	1.256	64207.8	971.05	1.3561	1.3065	1.3757	1.3748	1.348	1.285	1.405	1.4167
4.0	0.2806	46320.3	188.71	0.300	0.2912	0.3439	0.3961	0.4706	0.304	0.4399	0.537
5.0	0.0398	24983.2	28.723	0.0385	0.0509	0.0547	0.0964	0.155	0.041	0.065	0.069

Distance x in m	Exact solution	$\theta = 0.875$			$\theta = 1.0$		
		$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$
0.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
1.0	7.138	7.098	6.896	8.396	7.0465	6.757	6.306
2.0	3.649	3.704	3.554		3.668	3.4908	3.279
3.0	1.256	1.4012	1.446		1.417	1.482	1.554
4.0	0.2806	0.393	0.4984		0.4204	0.55	0.698
5.0	0.0398	0.085	0.153		0.0199	0.104	0.197

contd...

Table 2 (continued). COMPARISON OF RESULTS FOR LINEAR ELEMENTS AFTER 15 MINUTES

Distance x in m	Exact solution	$\theta = 0.0$	$\theta = 0.5$	$\theta = 2/3$		$\theta = 0.75$		$\theta = 0.875$	$\theta = 1.0$	
		$\Delta t = 2.51$	$\Delta t = 2.5$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 2.5$	$\Delta t = 2.5$	$\Delta t = 5.0$
0.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
1.0	8.1598	279672.8	8.291	8.1283	8.005	8.175	7.954	7.992	6.552	7.591
2.0	5.4641	330276.9	5.6249	5.451	5.374	5.4815	5.219	5.281	3.935	4.877
3.0	2.8738	184753.4	2.981	2.933	2.840	2.9133	2.824	2.889	2.021	2.793
4.0	1.153	62877.07	1.2026	1.267	1.278	1.1981	1.341	1.3409	0.9156	1.479
5.0	0.3463	15315.31	0.3606	0.451	0.5185	0.3907	0.41225	0.4056	0.3752	0.74
6.0	0.0769	2975.391	0.0853	0.1376	0.1961	0.08159	0.0956	0.07915	0.1418	0.355
7.0	0.0125	493.0508	0.01694	0.037	0.0705	0.0156	0.0169	0.0158	0.0503	0.165

contd...

Table 2 (continued). COMPARISON OF RESULTS FOR QUADRATIC ELEMENTS AFTER 5 MINUTES

Distance x in m	Exact solution	$\theta = 0.0$			$\theta = 0.5$				$\theta = 2/3$			
		$\Delta t = 0.5$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 0.5$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 0.5$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$
0.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
1.0	4.9014	0.185×10^{10}	-1028507	612.62	4.923	4.877	5.224	4.197	4.850	4.7966	4.684	4.579
2.0	1.1269	0.1647×10^{10}	-311661	37.05	1.1256	1.1076	0.9694	0.8809	1.141	1.1446	1.127	1.1089
3.0	0.1088	0.645×10^{9}	-40131.3	-0.285	0.211	0.20847	0.225	0.2732	0.133	0.1564	0.2195	0.3014

Distance x in m	Exact solution	$\theta = 0.75$				$\theta = 0.875$				$\theta = 1.0$		
		$\Delta t = 0.5$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 0.5$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$
0.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
1.0	4.9014	4.9174	4.7334	4.5056	3.988	4.7689	4.6389	4.2991	4.7211	4.5495	4.140	3.682
2.0	1.1269	1.1498	1.1634	1.1822	1.1919	1.1628	1.1904	1.2463	1.1757	1.2153	1.2958	1.354
3.0	0.1088	0.1445	0.177	0.2586	0.3562	0.1609	0.2060	0.3127	0.1765	0.239	0.3615	0.498

contd...

Table 2 (continued). COMPARISON OF RESULTS FOR QUADRATIC ELEMENTS AFTER 10 MINUTES

Distance x in m	Exact solution	$\theta = 0.0$		$\theta = 0.50$			$\theta = 2/3$			$\theta = 0.75$		
		$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$
0.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
1.0	7.1379	0.316×10^{13}	2260186	7.1982	7.049	8.164	7.0777	6.9975	7.1369	7.141	6.9115	6.8124
2.0	3.6498	0.265×10^{13}	431399	3.654	3.691	3.421	3.601	3.524	3.3232	3.6761	3.4684	3.276
3.0	1.2563	0.974×10^{12}	39717.9	1.2511	1.1992	1.0763	1.2778	1.286	1.2291	1.2910	1.3222	1.3498
4.0	0.2806	0.2148×10^{12}	2663.4	0.2795	0.2776	0.3011	0.3222	0.3752	0.4499	0.302	0.4173	0.5142
5.0	0.0398	0.333×10^{11}	149.43	0.0418	0.052	0.07898	0.0606	0.0944	0.1500	0.0499	0.1158	0.1868

Distance x in m	Exact solution	$\theta = 0.875$		$\theta = 1.0$		
		$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 1.0$	$\Delta t = 2.5$	$\Delta t = 5.0$
0.0	10.0	10.0	10.0	10.0	10.0	10.0
1.0	7.1379	6.9854	6.765	6.9287	6.6139	6.1362
2.0	3.6498	3.5411	3.4014	3.5088	3.3476	3.1604
3.0	1.2563	1.3105	1.3694	1.3295	1.4103	1.4948
4.0	0.2806	0.37007	0.4739	0.396	0.5244	0.6271
5.0	0.0398	0.0838	0.1475	0.0976	0.1785	0.2922

contd...

Table 2 (continued). COMPARISON OF RESULTS FOR QUADRATIC ELEMENTS AFTER 15 MINUTES

Distance x in m	Exact solution	$\theta = 0.0$	$\theta = 0.5$		$\theta = 2/3$		$\theta = 0.75$		$\theta=0.875$	$\theta = 1.0$	
		$\Delta t = 2.5$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 2.5$	$\Delta t = 5.0$	$\Delta t = 2.5$	$\Delta t = 2.5$	$\Delta t = 5.0$
0.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
1.0	8.1598	0.5895×10^{10}	8.0777	7.7632	8.073	7.992	8.2181	7.906	7.9288	7.8346	7.4967
2.0	5.4642	0.2335×10^{10}	5.4854	5.7063	5.3362	5.2439	5.4653	5.0922	5.1645	5.0709	4.1745
3.0	2.8738	0.384×10^{9}	2.8632	2.7478	2.8107	2.729	2.8934	2.7232	2.7861	2.7734	2.7124
4.0	1.153	0.408×10^{8}	1.1283	1.0478	1.2034	0.9849	1.2372	1.2883	1.2834	1.3249	1.4323
5.0	0.3463	333405.4	0.3421	0.3493	0.4301	0.3936	0.4686	0.5612	0.5213	0.5691	0.7167
6.0	0.0769	229098.5	0.08485	0.1069	0.1336	0.1479	0.1573	0.2307	0.1473	0.1761	0.2854

CHAPTER 5

SUMMARY, CONCLUSIONS AND SUGGESTIONS FOR FURTHER WORK

5.1. Summary:

In water resources development and management one of the main problem is that of water quality. While discussing the water quality problem the question of transport and accumulation of pollutant in an aquifer needs special attention. Though it seems that groundwater is more protected against pollution than surface water but when groundwater is polluted, it is very difficult to bring it back to its original state.

Most of the groundwater becomes polluted by the pollutants brought down from the surface. Under natural conditions an equilibrium exists between the water leaving the formation and pollutant which is carried with this water. When an aquifer is recharged with an inferior quality water or with water having more pollutant concentration than that already present in the aquifer, this equilibrium is destroyed. The equilibrium is restored again after a rise in pollutant concentration in the aquifer. Sometimes this new pollutant concentration may go beyond the permissible limits, thus causing pollution problem.

The sources of groundwater pollution may be the following. Flow of water through carbonate rocks, sea water intrusion into aquifer, accidental breaking of sewers loading to discharge of inferior quality water into the aquifer and percolation from septic tank. Sometimes rain water and irrigation water carrying

the fertilizer salts, herbicides and pesticides may infiltrate through the ground surface polluting the aquifer. After studying the various causes of pollution of groundwater it becomes essential to have methods for prediction of the distribution of the pollutant in the groundwater.

In the present study an attempt has been made to study the pollutant transport in groundwater flowing through porous media. The spread of pollutant in groundwater takes place in many different ways like mechanical dispersion, molecular diffusion, hydrodynamic dispersion etc. Also other phenomena like adsorption, radioactive decay etc. may affect the pollutant transport phenomena. So suitable mathematical models need to be developed including all the above mechanisms in order to suitably represent the actual conditions. Keeping this in view a suitable mathematical model has been developed to adequately describe the pollutant transport phenomena in the groundwater. The resulting differential equations both for one dimensional and two dimensional cases were solved using finite element technique.

To solve the dispersion equation for pollutant transport in one dimensional flow field, both linear and quadratic elements have been taken for Galerkin Finite Element solution. Special cases of same problem were solved analytically and results were compared with finite element solution. The results match closely. Further, the solution of dispersion equation was done by varying various parameters like R, λ, q, c^* and results are plotted and analysed. It is noted that if the value of λ is low then its effect on concentration profile is negligible. Also the

volumetric fluid injection rate and concentration of source of fluid affect the pollutant concentration at a distance far away from the source. It is also seen that the results obtained by linear and quadratic elements give matching results.

For solving two dimensional dispersion equation in two dimensional flow field, two different sets of boundary conditions were considered. Results obtained from the first set of boundary conditions are plotted in the form of concentration contours. These results indicate that near the impervious and concentration-specified edges, concentration gradients are high and this gradient increases with increase in time interval. In the middle of the domain the concentration is nearly constant. Its value decreases with increase in time.

5.2. Conclusions:

The following conclusions may be drawn from the results obtained by solving one dimensional and two dimensional pollutant transport equations by finite element method.

(i) During finite element formulation of the problem, the value of θ was varied over a range of 0 to 1. It is found that for $\theta = 0.75$ the finite element results match closely with the analytical results.

(ii) For radioactive pollutant of higher half life period like radium etc., radioactive decay does not affect significantly the pollutant distribution in the aquifer.

(iii) An increase in retardation factors (considering adsorption) leads to lesser over all pollutant concentration in the aquifer.

(iv) Groundwater recharge with pollutant concentration will have considerable effect on the over all pollutant concentration in the aquifer.

(v) In two dimensional case the concentration contours vary greatly depending on the boundary conditions with concentration gradients vary high near impervious and concentration specified boundaries. In the middle portion of the domain in two dimensional cases, the concentration has been found to be nearly constant and the concentration gradients small.

Some of the limitations of the study are: (1) ion-exchange phenomena was not included, (2) three dimensional aspects of the study were not considered and (3) only single boundary conditions and triangular elements were used in the finite element formulation in two-dimensional case.

5.3. Suggestion for Further Work:

Following are a few suggestions that can be incorporate in further work:

(1) Two dimensional case results can be obtained for different boundary conditions and for different values of R, q, c^* and λ. Further, 8 noded isoparametric elements can be taken to solve the same governing differential equation to give better results.

(2) Ion-exchange phenomena should be included in the governing differential equations. A program can be developed for three dimensional dispersion equation. In this case it must be kept in mind that this involves a lot of computer memory space and execution time.

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APPENDIX A

DERIVATION OF THE GOVERNING DIFFERENTIAL EQUATION

A.1. Fick's First Law of Binary Diffusion:

Consider a small volume of mixture of fluids A and B. Let c_A and c_B be the mass of A and B per unit volume of the mixture. Let $\overline{V}_A$ and $\overline{V}_B$ be their respective average velocities. Then for the mixture

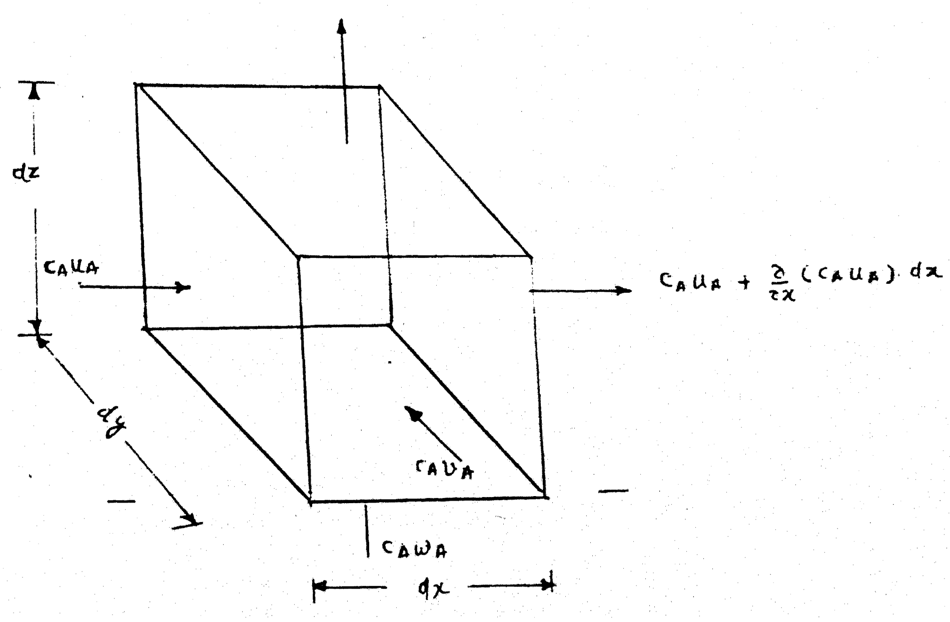
$$c = c_A + c_B \quad \text{and velocity} \quad V = \frac{c_A\overline{V}_A + c_B\overline{V}_B}{c} \tag{A.1}$$

Thus for an isotropic material, Fick's law of binary diffusion relates the motion of A, relative to average motion of mixture, to concentration gradient

$$c_A(\overline{V}_A - \overline{V}) = - c\, D_m \text{ grad } (\frac{c_A}{c}) \tag{A.2}$$

where D_m = coefficient of molecular dispersion of the mixture. Similar equation can be written for material B.

A.2. Derivation of the Differential Equation:



Consider an elemental volume as shown above. Now

$$\overline{V}_A = i\ u_A + j\ v_A + k\ w_A$$

Mass of pollutant entering the elemental volume in x direction in time dt = $(c_A u_A)$ dy dz dt.

Mass of pollutant leaving the elemental volume in x direction in time dt

$$= c_A u_A + \left[\frac{\partial}{\partial x}(c_A u_A)\,dx\right] dy\ dz\ dt$$

Net amount of pollutant which enters elemental volume in x direction

$$= (c_A u_A)\,dy\ dz\ dt - \left[c_A u_A + \frac{\partial}{\partial x}(c_A u_A)\,dx\right] dy\ dz\ dt$$

$$= -\frac{\partial}{\partial x}(c_A u_A)\ dx\ dy\ dz\ dt$$

Similarly net amount of pollutant which enters in elemental volume in y direction

$$= -\frac{\partial}{\partial y}(c_A v_A)\ dx\ dy\ dz\ dt$$

Net amount of pollutant entered into elemental volume in z direction

$$= -\frac{\partial}{\partial z}(c_A w_A)\ dx\ dy\ dz\ dt$$

Net increase of mass

$$= \left(\frac{\partial c_A}{\partial t}\ dt\right) n\ dx\ dy\ dz + \left(\frac{\partial s}{\partial t}\ dt\right)(1-n)\ dx\ dy\ dz$$

where n = porosity

s = mass of pollutant adsorbed per unit volume of the porous medium.

Mass balance equation, when no chemical change is involved, is:

Net mass out flow in x direction	+	Net mass out flow in y direction	+	Net mass out flow in z direction	+	Added mass	-	Mass decayed

= Increase of mass

$$-\left[\frac{\partial}{\partial x}(c_A u_A) + \frac{\partial}{\partial y}(c_A v_A) + \frac{\partial}{\partial z}(c_A w_A)\right] dx\, dy\, dz\, dt + qc \quad dx\, dy\, dz\, dt$$

$$- \lambda\left[nc_A + (1-n)s\right] dx\, dy\, dz\, dt$$

$$= \left[n\frac{\partial c_A}{\partial t} + (1-n)\frac{\partial s}{\partial t}\right] dx\, dy\, dz\, dt$$

where c^* = concentration of source fluid

q = volumetric fluid injection rate.

i.e.

$$- \frac{\partial}{\partial x}\left[(c_A u_A) + \frac{\partial}{\partial y}(c_A v_A) + \frac{\partial}{\partial z}(c_A w_A)\right] + qc^* - \lambda\left[nc_A + (1-n)s\right]$$

$$= n\frac{\partial c_A}{\partial t} + (1-n)\frac{\partial s}{\partial t}$$

$$- \operatorname{div}(c_A . \overline{V}_A) + qc^* - \lambda\left[nc_A + (1-n)s\right] = n\frac{\partial c_A}{\partial t} + (1-n)\frac{\partial s}{\partial t} \tag{A.3}$$

From Fick's law

$$\frac{c_A}{n}(\overline{V}_A - \overline{V}) = - c\, D\, \mathrm{grad}\left(\frac{c_A}{c}\right)$$

Taking D as a dispersion tensor and c average density of mixture, as constant

$$c_A \overline{V}_A = c_A \overline{V} - n\, D\, \mathrm{grad}(c_A)$$

Now substituting $c_A \overline{V}_A$ in (A.3), we get

$$- \operatorname{div} [c_A \overline{V} - n\, D \operatorname{grad}(c_A)] - \lambda [n c_A + (1-n) s] + q c^* = n \frac{\partial c_A}{\partial t} + (1-n) \frac{\partial s}{\partial t}$$

or

$$n \frac{\partial c_A}{\partial t} + (1-n) \frac{\partial s}{\partial t} = \operatorname{div} [n\, D \operatorname{grad}(c_A) - c_A \overline{V}] - \lambda [n c_A + (1-n) s] + q c^*$$

Now dropping c_A as c we get

$$n \frac{\partial c}{\partial t} + (1-n) \frac{\partial s}{\partial t} = \operatorname{div} [n\, D \operatorname{grad}(c) - c\overline{V}] - \lambda [n c + (1-n) s] + q c^*$$

In tensor notation, equation can be written as

$$n \frac{\partial c}{\partial t} + (1-n) \frac{\partial s}{\partial t} = \frac{\partial}{\partial x_i} [n\, D_{ij} \frac{\partial}{\partial x_j} - c u_i] - \lambda [n c + (1-n) s] + q c^* .$$

APPENDIX B

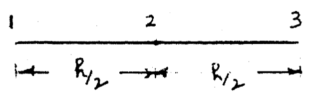
TO FIND SHAPE FUNCTIONS

B.1. For Quadratic Element:

Let the solution over element for the quadratic interpolation model be expressed as

$$c^{(e)}(x, t) = \alpha_1 + \alpha_2 x + \alpha_3 x^2 \qquad (B.1)$$

where α_1, α_2 and α_3 are the functions of time t. Since there are three constants α_1, α_2, α_3 in equation (B.1), the element is assumed to have three degree of freedom, one at each end and one at middle point.



Let

$$c^{(e)}(x, t) = \varphi_1 \text{ at } x = 0$$

$$c^{(e)}(x, t) = \varphi_2 \text{ at } x = h/2$$

$$c^{(e)}(x, t) = \varphi_3 \text{ at } x = h$$

where all φ's are the functions of time, t.

From (B.1), substituting the values of φ_1, φ_2, φ_3 for various values of x we get

$$\alpha_1 = \varphi_1$$

$$\varphi_2 = \varphi_1 + \alpha_2 \frac{h}{2} + \alpha_3 \frac{h^2}{4}$$

$$\varphi_3 = \varphi_1 + \alpha_2 h + \alpha_3 h^2$$

$$\alpha_2 = (4\varphi_2 - 3\varphi_1 - \varphi_3)/h$$

$$\alpha_3 = 2(\varphi_1 - 2\varphi_2 + \varphi_3)/h^2$$

by substituting values of α_1, α_2, α_3 in equation (B.1) we get

$$c^{(e)}(x,\ t) = \varphi_1 + (4\varphi_2 - 3\varphi_1 - \varphi_3)\frac{x}{h} + 2(\varphi_1 - 2\varphi_2 + \varphi_3)\frac{x^2}{h^2}$$

$$= (1 - \frac{3x}{h} + \frac{2x^2}{h^2})\varphi_1 + (\frac{4x}{h} - \frac{4x^2}{h^2})\varphi_2 - (\frac{x}{h} - \frac{2x^2}{h^2})\varphi_3$$

$$= (1 - \frac{x}{h})(1 - \frac{2x}{h})\varphi_1 + \frac{4x}{h}(1 - \frac{x}{h})\varphi_2 - \frac{x}{h}(1 - \frac{2x}{h})\varphi_3$$

$$= \lfloor N_1(x),\ N_2(x),\ N_3(x) \rfloor \begin{Bmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{Bmatrix} \qquad \text{(B.2)}$$

$$= \lfloor N(x) \rfloor \ \{\varphi\}^{(ne)}$$

where

$$N(x) = \lfloor N_1(x),\ N_2(x),\ N_3(x) \rfloor$$

$$N_1(x) = (1 - \frac{x}{h})(1 - \frac{2x}{h})$$

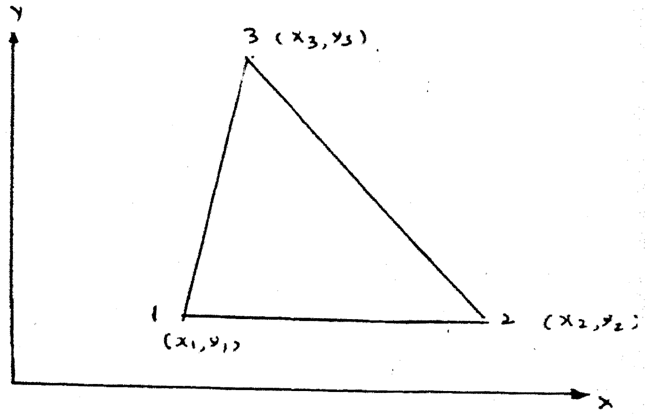
$$N_2(x) = \frac{4x}{h}(1 - \frac{x}{h})$$

$$N_3(x) = -\frac{x}{h}(1 - \frac{2x}{h})$$

and $\{\varphi\}^{(ne)} = \begin{Bmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{Bmatrix}$

B.2. <u>For Triangular Element:</u>

The two dimensional simplex element is a straight sided triangle with three nodes one at each corner as shown in figure. Let the nodes are labelled as 1, 2 and 3 in anticlockwise direction.



We assume a linear variation of concentration c inside the element

$$c^{(e)}(x, y, t) = \alpha_1 + \alpha_2 x + \alpha_3 y \tag{B.3}$$

where α_1, α_2, α_3 are the functions of time.

By using nodal conditions i.e.

$$c^{(e)}(x_1, y_1, t) = \varphi_1(t) \quad \text{at node 1 } (x_1, y_1)$$

$$c^{(e)}(x_2, y_2, t) = \varphi_2(t) \quad \text{at node 2 } (x_2, y_2)$$

$$c^{(e)}(x_3, y_3, t) = \varphi_3(t) \quad \text{at node 3 } (x_3, y_3)$$

lead to system of equations

$$\varphi_1 = \alpha_1 + \alpha_2 x_1 + \alpha_3 y_1 \tag{B.4}$$

$$\varphi_2 = \alpha_1 + \alpha_2 x_2 + \alpha_3 y_2 \tag{B.5}$$

$$\varphi_3 = \alpha_1 + \alpha_2 x_3 + \alpha_3 y_3 \tag{B.6}$$

The solution of above equations yield

$$\alpha_1 = \frac{1}{2A^{(e)}} (a_1\varphi_1 + a_2\varphi_2 + a_3\varphi_3)$$

$$\alpha_2 = \frac{1}{2A^{(e)}} (b_1\varphi_1 + b_2\varphi_2 + b_3\varphi_3)$$

$$\alpha_3 = \frac{1}{2A^{(e)}} (c_1\varphi_1 + c_2\varphi_2 + c_3\varphi_3)$$

where $A^{(e)}$ is the area of triangular element 123, given by

$$A^{(e)} = \frac{1}{2} (x_1y_2 + x_2y_3 + x_3y_1 - y_1x_2 - y_2x_3 - y_3x_1)$$

and

$$a_1 = x_2y_3 - x_3y_2 \qquad b_1 = y_2 - y_3 \qquad c_1 = x_3 - x_2$$

$$a_2 = x_3y_1 - x_1y_3 \qquad b_2 = y_3 - y_1 \qquad c_2 = x_1 - x_3$$

$$a_3 = x_1y_2 - x_2y_1 \qquad b_3 = y_1 - y_2 \qquad c_3 = x_2 - x_1$$

On the substitution of the values α_1, α_2, α_3 in equation (B.3) and rearranging the terms, we get

$$\begin{aligned} c^{(e)}(x, y, t) &= N_1(x, y)\varphi_1 + N_2(x, y)\varphi_2 + N_3(x, y)\varphi_3 \qquad \text{(B.7)} \\ &= \lfloor N(x, y) \rfloor \{\varphi(t)\}^{(ne)} \end{aligned}$$

where $\lfloor N(x, y) \rfloor = \lfloor N_1(x, y), N_2(x, y), N_3(x, y) \rfloor$

$$N_1(x, y) = \frac{1}{2A^{(e)}} (a_1 + b_1x + c_1y)$$

$$N_2(x, y) = \frac{1}{2A^{(e)}} (a_2 + b_2x + c_2y)$$

$$N_3(x, y) = \frac{1}{2A^{(e)}} (a_3 + b_3x + c_3y)$$

and $$\{\varphi(t)\}^{(ne)} = \begin{Bmatrix} \varphi_1(t) \\ \varphi_2(t) \\ \varphi_3(t) \end{Bmatrix} .$$

```
C        MAIN PROGRAM FOR LINEAR ELEMENTS
C*************************************************************************
C        CORD=MATRIX STORING X AND Y CORDINATES OF NODES
C        KONECT=KONECTIVITY MATRIX FOR VARIOUS ELEMENTS
C        ELGK=ELEMENTAL [K] MATRIX
C        ELF=ELEMENTAL {F} MATRIX
C        GLGK=GLOBAL [K] MATRIX
C        GLF=GLOBAL {F} MATRIX
C        NNOD=NUMBER OF NODES
C        NELEM=NUMBER OF ELEMENTS
C        NSPCO=NUMBER OF NODES AT WHICH CONCENTRATION IS SPECIFIED
C        ISPCO=NODE NUMBERS AT WHICH CONCENTRATION IS SPECIFIED
C        SPCO= VALUES OF SPECIFIED CONCENTRATION
C        UX=DARCY'S VELOCITY VECTOR IN X-DIRECTION
C        DXX=DISPERSION COEFICIENT IN X-DIRECTION
C        POR=POROSITY
C        RETA=RETARDATION FACTOR(R)
C        DT=TIME INTERVAL
C        Q=VOLUMETRIC FLUID INJECTION RATES
C        CST=CONCENTRATION OF SOURCE FLUID
C*************************************************************************
C        COMMON/A1/CORD(NNOD,2),NNOD
C        COMMON/A2/KONECT(NELEM,2),NELEM
C        COMMON/A3/ELGK(2,2),ELF(2)
C        COMMON/A4/DXX,RETA,CST,XAMD,Q,UX,POR,DT
C        COMMON/A5/CONC(NNOD)
C        COMMON/A6/GLGK(NNOD,NNOD),GLF(NNOD)
C        COMMON/A7/NSPCO,ISPC(2),SPCO(2)
         COMMON/A1/CORD(101,2),NNOD
         COMMON/A2/KONECT(100,2),NELEM
         COMMON/A3/ELGK(2,2),ELF(2)
         COMMON/A4/DXX,RETA,CST,XLAMD,Q,UX,POR,DT
         COMMON/A5/CONC(101)
         COMMON/A6/GLGK(101,101),GLF(101)
         COMMON/A7/NSPCO,ISPCO(2),SPCO(2)
         DATA DXX,RETA,CST,XLAMD,Q,UX,POR,DT/0.1,1.0,0.0,0.0,0.0,0.039,
        1 0.39,0.5/
         DATA NSPCO,ISPCO,SPCO/2,1,101,10.0,0.0/
         DATA NNOD,NELEM/101,100/
         DO 1 I=1,NNOD
1        READ(23,*) (CORD(I,J),J=1,2),CONC(I)
         DO 2 I=1,NELEM
2        READ(23,*),(KONECT(I,J),J=1,2)
         T=0.0
         DO 3 I=1,10
         T=T+DT
         CALL ASMBL
         CALL SPCONC
         CALL GAUSJD(GLGK,GLF,NNOD)
         TYPE *,NNOD
         DO 49 J=1,NNOD
         CONC(J)=GLF(J)
49       WRITE(40,*),T,J,CONC(J)
3        CONTINUE
         STOP
         END
C*************************************************************************
         SUBROUTINE ELEM(IELEM)
         COMMON/A1/CORD(101,2),NNOD
         COMMON/A2/KONECT(100,2),NELEM
         COMMON/A3/ELGK(2,2),ELF(2)
         COMMON/A4/DXX,RETA,CST,XLAMD,Q,UX,POR,DT
         COMMON/A5/CONC(101)
         COMMON/A6/GLGK(101,101),GLF(101)
         COMMON/A7/NSPCO,ISPCO(2),SPCO(2)
         DIMENSION NODE(2),A(2,2),ELGP(2,2)
         DO 1 I=1,2
1        NODE(I)=KONECT(IELEM,I)
         H=0.0
         DO 2 I=1,2
2        H=H+(CORD(NODE(1),I)-CORD(NODE(2),I))**2
         H=SQRT(H)
         DO 3 I=1,2
         ELF(I)=0.0
         DO 3 J=1,2
         ELGK(I,J)=0.0
         ELGP(I,J)=0.0
3        CONTINUE
C        TO CALCULATE ELEMENTAL MATRICES
         ELGK(1,1)=DXX/(1.0*H)-UX/(2.0*POR)+(XLAMD*RETA*H)/3.0
         ELGK(1,2)=-DXX/(1.0*H)+UX/(2.0*POR)+(XLAMD*RETA*H)/6.0
         ELGK(2,1)=-DXX/(1.0*H)-UX/(2.0*POR)+(XLAMD*RETA*H)/6.0
         ELGK(2,2)=DXX/(1.0*H)+UX/(2.0*POR)+(XLAMD*RETA*H)/3.0
         ELGP(1,1)=(RETA*H)/(3.0*DT)
         ELGP(1,2)=(RETA*H)/(6.0*DT)
         ELGP(2,1)=(RETA*H)/(6.0*DT)
         ELGP(2,2)=(RETA*H)/(3.0*DT)
         ELF(1)=(Q*CST*H)/(2.0*POR)
         ELF(2)=(Q*CST*H)/(2.0*POR)
```

```
      DO 1 I=1,NNOD
1     GLF(I)=GLF(I)-SPCO(J)*GLGK(I,ISPCO(J))
      DO 3 I1=1,NSPCO
      I=ISPCO(I1)
      GLF(I)=SPCO(I1)
      DO 2 J=1,NNOD
      GLGK(I,J)=0.0
2     GLGK(J,I)=0.0
3     GLGK(I,I)=1.0
      RETURN
      END
```

```
C         MAIN PROGRAM FOR QADRATIC ELEMENTS
C         COMMON/A1/CORD(NNOD,2),NNOD
C         COMMON/A2/KONECT(NELEM,2),NELEM
C         COMMON/A3/ELGK(2,2),ELF(2)
C         COMMON/A4/DXX,RETA,CST,XLAMD,Q,UX,POR,DT
C         COMMON/A5/CONC(NNOD)
C         COMMON/A6/GLGK(NNOD,NNOD),GLF(NNOD)
          COMMON/A7/NSPCO,ISPC(2),SPCO(2)
          COMMON/A1/CORD(101,2),NNOD
          COMMON/A2/KONECT(50,3),NELEM
          COMMON/A3/ELGK(3,3),ELF(3)
          COMMON/A4/DXX,RETA,CST,XLAMD,Q,UX,POR,DT
          COMMON/A5/CONC(101)
          COMMON/A6/GLGK(101,101),GLF(101)
          COMMON/A7/NSPCO,ISPCO(2),SPCO(2)
          DATA DXX,RETA,CST,XLAMD,Q,UX,POR,DT/0.1,1.0,0.0,0.0,0.0,0.039,
          1 0.39,1.0/
          DATA NSPCO,ISPCO/2,1,101/
          DATA NNOD,NELEM/101,50/
          DATA SPCO/10.0,0.0/
          DO 1 I=1,NNOD
1         READ(21,*),(CORD(I,J),J=1,2),CONC(I)
          DO 2 I=1,NELEM
2         READ(21,*),(KONECT(I,J),J=1,3)
          T=0.0
          DO 3 I=1,10
          T=T+DT
          CALL ASMBL
          CALL SPCONC
          CALL GAUSJD(GLGK,GLF,NNOD)
          TYPE *,NNOD
          DO 49 J=1,NNOD
          CONC(J)=GLF(J)
49        WRITE(47,*),T,J,CONC(J)
3         CONITNUE
          STOP
          END
C***************************************************************************
          SUBROUTINE ELEM(IELEM)
          COMMON/A1/CORD(101,2),NNOD
          COMMON/A2/KONECT(50,3),NELEM
          COMMON/A3/ELGK(3,3),ELF(3)
          COMMON/A4/DXX,RETA,CST,XLAMD,Q,UX,POR,DT
          COMMON/A5/CONC(101)
          COMMON/A6/GLGK(101,101),GLF(101)
          COMMON/A7/NSPCO,ISPCO(2),SPCO(2)
          DIMENSION NODE(3),A(3,3),ELGP(3,3)
          DO 1 I=1,3
1         NODE(I)=KONECT(IELEM,I)
          H=0.0
          DO 2 I=1,2
2         H=H+(CORD(NODE(1),I)-CORD(NODE(3),I))**2
          H=SQRT(H)
          DO 3 I=1,3
          ELF(I)=0.0
          DO 3 J=1,3
          ELGK(I,J)=0.0
          ELGP(I,J)=0.0
3         CONTINUE
C         TO CALCULATE ELEMENTAL MATRICES
          ELGK(1,1)=(7*DXX)/(3.0*H)-UX/(2.0*POR)+(XLAMD*RETA*H*2.0)/15.0
          ELGK(1,2)=-(8.0*DXX)/(3.0*H)+UX/(1.5*POR)+(XLAMD*RETA*H)/15.0
          ELGK(1,3)=DXX/(3.0*H)-UX/(6.0*POR)-(XLAMD*RETA*H)/30.0
          ELGK(2,1)=-(8.*DXX)/(3.0*H)-UX/(1.5*POR)+(XLAMD*RETA*H)/15.0
          ELGK(2,2)=(16.0*DXX)/(3.0*H)+(8.0*XLAMD*RETA*H)/15.0
          ELGK(2,3)=-(8.*DXX)/(3.0*H)+UX/(1.5*POR)+(XLAMD*RETA*H)/15.0
          ELGK(3,1)=DXX/(3.0*H)+UX/(6.0*POR)-(XLAMD*RETA*H)/30.0
          ELGK(3,2)=-(8.0*DXX)/(3.0*H)-UX/(1.5*POR)+(XLAMD*RETA*H)/15.0
          ELGK(3,3)=(7.0*DXX)/(3.0*H)+UX/(2.0*POR)+(2.0*XLAMD*RETA*H)/15.0
          ELGP(1,1)=(RETA*H)/(7.5*DT)
          ELGP(1,2)=(RETA*H)/(15.0*DT)
          ELGP(1,3)=-(RETA*H)/(30.0*DT)
          ELGP(2,1)=(RETA*H)/(15.0*DT)
          ELGP(2,2)=(8.0*RETA*H)/(15.0*DT)
          ELGP(2,3)=(RETA*H)/(15.0*DT)
          ELGP(3,1)=-(RETA*H)/(30.0*DT)
          ELGP(3,2)=(RETA*H)/(15.0*DT)
          ELGP(3,3)=(2*RETA*H)/(15.0*DT)
          ELF(1)=(Q*CST*H)/(6.0*POR)
          ELF(2)=(Q*CST*H)/(6.0*POR)
          ELF(3)=(Q*CST*H)/(6.0*POR)
          TH=0.875
          DO 5 I=1,3
          DO 5 J=1,3
          A(I,J)=(ELGP(I,J)-((1-TH)*ELGK(I,J)))
          ELGK(I,J)=(ELGP(I,J)+TH*ELGK(I,J))
5         CONTINUE
          DO 6 I=1,3
          DO 6 J=1,3
```

```
      ELF(I)=ELF(I)+A(I,J)*CONC(KONECT(IELEM,J))
6     CONTINUE
      RETURN
      END
C ***********************************************************************
      SUBROUTINE ASMBL
      COMMON/A1/CORD(101,2),NNOD
      COMMON/A2/KONECT(50,3),NELEM
      COMMON/A3/ELGK(3,3),ELF(3)
      COMMON/A4/DXX,RETA,CST,XLAMD,Q,UX,POR,DI
      COMMON/A5/CONC(101)
      COMMON/A6/GLGK(101,101),GLF(101)
      COMMON/A7/NSPCO,ISPCO(2),SPCO(2)
      DO 1 I=1,NNOD
      GLF(I)=0.0
      DO 1 J=1,NNOD
      GLGK(I,J)=0.0
1     CONTINUE
      DO 2 I=1,NELEM
      IELEM=I
      CALL ELEM(IELEM)
      DO 2 J=1,3
      GLF(KONECT(IELEM,J))=GLF(KONECT(IELEM,J))+ELF(J)
      DO 2 K=1,3
      GLGK(KONECT(IELEM,J),KONECT(IELEM,K))=GLGK(KONECT(IELEM,J),
     1KONECT(IELEM,K))+ELGK(J,K)
2     CONTINUE
      RETURN
      END
C***********************************************************************
      SUBROUTINE GAUSJD(A,C,N)
      DIMENSION A(101,101),C(101)
      DO 1 I=1,N
      BIG=ABS(A(1,I));INDBIG=1
      NI1=N-I+1;IF(NI1.LT.2) GO TO 3
      DO 2 J=2,NI1
      IF(ABS(A(J,I)).LE.BIG) GO TO 2
      BIG=ABS(A(J,I));INDBIG=J
2     CONTINUE
      IF(INDBIG.EQ.1) GO TO 3
      T=C(INDBIG);C(INDBIG)=C(1);C(1)=T
      DO 3 K=1,N
      T=A(INDBIG,K);A(INDBIG,K)=A(1,K);A(1,K)=T
3     CONTINUE
      IP1=I+1
      IF(IP1.GT.N) GO TO 13
      DO 5 KL=IP1,N
5     A(1,KL)=A(1,KL)/A(1,I)
13    C(1)=C(1)/A(1,I)
      A(1,I)=1.
      DO 9 LM=2,N
      C(LM)=C(LM)-C(1)*A(LM,I)

      IF(IP1.GT.N) GO TO 9
      IF(A(LM,I).EQ.0.0) GO TO 4
      DO 4 L=IP1,N
      A(LM,L)=A(LM,L)-A(1,L)*A(LM,I)
4     CONTINUE

9     A(LM,I)=A(LM,I)-A(1,I)*A(LM,I)
15    TC=C(1)
      DO 7 MN=1,N
      T=A(1,MN)
      IF(MN.GT.1) C(MN-1)=C(MN)
      DO 6 NO=2,N
6     A(NO-1,MN)=A(NO,MN)
7     A(N,MN)=T
      C(N)=TC
1     CONTINUE
      RETURN
      END
C***********************************************************************
      SUBROUTINE SPCONC
      COMMON/A1/CORD(101,2),NNOD
      COMMON/A2/KONECT(50,3),NELEM
      COMMON/A3/ELGK(3,3),ELF(3)
      COMMON/A4/DXX,RETA,CST,XLAMD,Q,UX,POR,DI
      COMMON/A5/CONC(101)
      COMMON/A6/GLGK(101,101),GLF(101)
      COMMON/A7/NSPCO,ISPCO(2),SPCO(2)
      DO 1 J=1,NSPCO
      DO 1 I=1,NNOD
1     GLF(I)=GLF(I)-SPCO(J)*GLGK(I,ISPCO(J))
      DO 3 I1=1,NSPCO
      I=ISPCO(I1)
      GLF(I)=SPCO(I1)
      DO 2 J=1,NNOD
      GLGK(I,J)=0.0
2     GLGK(J,I)=0.0
```

```
3       GLGK(I,I)=1.0
        RETURN
        END
```

```
C*********************************************************************
C        NBOND= NUMBER OF BOUNDARY NODES
C        IBOND=MATRIX SHOWING ITS ELEMENT NUMBER AND IT'S BOUNDARY NODES
C*********************************************************************
C        MAIN PROGRAM FOR TWO DIMENSIONAL CASE
         COMMON/A1/CORD(147,2),NNOD
         COMMON/A2/KONECT(240,3),NELEM
         COMMON/A3/ELGK(3,3),ELF(3),LOCNOD(2),D(3,3),E(3)
         COMMON/A4/DXX,DXY,DYX,DYY,RETA,CST,XLAMD,Q,UX,UY,POR,DT,ALPH
         COMMON/A5/CONC(147)
         COMMON/A6/NBOND,IBOND(20,3)
         COMMON/A7/GLGK(147,147),GLF(147)
         COMMON/A8/NSPCO,ISPCO(14),SPCO(14)
         DATA DXX,DXY,DYX,DYY,RETA,CST,XLAMD,Q,UX,UY,POR,DT,ALPH/
         1 .00006,0.0,0.0,.000009,1.0,0.0,0.0,0.0,.06,.012,.39,1.0,.1/
         DATA NNOD,NELEM/147,240/
         DATA NSPCO,ISPCO/14,1,22,43,64,85,106,127,21,42,63,84,105,126
         1,147/
         DATA SPCO/5.,5.,5.,5.,5.,5.,5.,0.0,0.0,0.0,0.0,0.0,0.0,0.0/
         DATA NBOND/20/
         DO 1 I=1,NNOD
1        READ(22,*)(CORD(I,J),J=1,2),CONC(I)
         DO 2 I=1,NELEM
2        READ(22,*)(KONECT(I,J),J=1,3)
         DO 11 I=1,NBOND
         READ(22,*),(IBOND(I,J),J=1,3)
11       CONTINUE
         T=0.0
         DO 3 I=1,50
         T=T+DT
         CALL ASMBL
         CALL SPCONC
         CALL GAUS JD(GLGK,GLF,NNOD)
         TYPE *,NNOD
         DO 49 J=1,NNOD
         CONC(J)=GLF(J)
49       WRITE(43,*) J,CONC(J)
3        CONTINUE
12       CONTINUE
         STOP
         END
C*********************************************************************
         SUBROUTINE SPCONC
         COMMON/A1/CORD(147,2),NNOD
         COMMON/A2/KONECT(240,3),NELEM
         COMMON/A3/ELGK(3,3),ELF(3),LOCNOD(2),D(3,3),E(3)
         COMMON/A4/DXX,DXY,DYY,DYY,RETA,CSI,XLAMD,Q,UX,UY,POR,DT,ALPH
         COMMON/A5/CONC(147)
         COMMON/A6/NBOND,IBOND(20,3)
         COMMON/A7/GLGK(147,147),GLF(147)
         COMMON/A8/NSPCO,ISPCO(14),SPCO(14)
         DO 1 J=1,NSPCO
         DO 1 I=1,NNOD
1        GLF(I)=GLF(I)-SPCO(J)*GLGK(I,ISPCO(J))
         DO 3 I1=1,NSPCO
         I=ISPCO(I1)
         GLF(I)=SPCO(I1)
         DO 2 J=1,NNOD
         GLGK(I,J)=0.0
2        GLGK(J,I)=0.0
3        GLGK(I,I)=1.0
         RETURN
         END
C*********************************************************************
         SUBROUTINE SURFAC(INOD1,JNOD1)
         COMMON/A1/CORD(147,2),NNOD
         COMMON/A2/KONECT(240,3),NELEM
         COMMON/A3/ELGK(3,3),ELF(3),LOCNOD(2),D(3,3),E(3)
         COMMON/A4/DXX,DXY,DYX,DYY,RETA,CSI,XLAMD,Q,UX,UY,POR,DT,ALPH
         COMMON/A5/CONC(147)
         COMMON/A6/NBOND,IBOND(20,3)
         COMMON/A7/GLGK(147,147),GLF(147)
         COMMON/A8/NSPCO,ISPCO(14),SPCO(14)
         DIMENSION S(2,2),P(2)
C         WRITE(20,*),LOCNOD(1),LOCNOD(2)
C        I=IBOND(IELEM,2)
C        J=IBOND(IELEM,3)
         B=CORD(INOD1,2)-CORD(JNOD1,2)
         C=CORD(JNOD1,1)-CORD(INOD1,1)
         S(1,1)=-(DXX-((B/C)*DYX))/2.0+((UX*C)-(UY*B))/(3.0*POR)
         S(1,2)=(DXX-((B/C)*DYX))/2.0+((UX*C)-(UY*B))/(6.0*POR)
         S(2,1)=-(DXX-((B/C)*DYX))/2.0+((UX*C)-(UY*B))/(6.0*POR)
         S(2,2)=(DXX-((B/C)*DYX))/2.0+((UX*C)-(UY*B))/(3.0*POR)
         P(1)=(ALPH/2.0)*((DXY*C)-(DYY*B))
         P(1)=(ALPH/2.0)*((DXY*C)-(DYY*B))
         DO 21 II=1,3
         E(II)=0.0
         DO 21 JJ=1,3
         D(II,JJ)=0.0
```

```
21        CONTINUE
          DO 7 L=1,2
          LL=LOCNOD(L)
          E(LL)=E(LL)+P(L)
          DO 7 M=1,2
          MM=LOCNOD(M)
          D(LL,MM)=D(LL,MM)+S(L,M)
7         CONTINUE
          RETURN
          END
C*****************************************************************************
          SUBROUTINE GAUSJD(A,C,N)
          DIMENSION A(147,147),C(147)
          DO 1 I=1,N
          BIG=ABS(A(1,I));INDBIG=1
          NI1=N-I+1;IF(NI1.LT.2) GO TO 3
          DO 2 J=2,NI1
          IF(ABS(A(J,I)).LE.BIG) GO TO 2
          BIG=ABS(A(J,I));INDBIG=J
2         CONTINUE
          IF(INDBIG.EQ.1) GO TO 3
          T=C(INDBIG);C(INDBIG)=C(1);C(1)=T
          DO 3 K=1,N
          T=A(INDBIG,K);A(INDBIG,K)=A(1,K);A(1,K)=T
3         CONTINUE
          IP1=I+1
          IF(IP1.GT.N) GO TO 13
          DO 5 KL=IP1,N
5         A(1,KL)=A(1,KL)/A(1,I)
13        C(1)=C(1)/A(1,I)
          A(1,I)=1.
          DO 9 LM=2,N
          C(LM)=C(LM)-C(1)*A(LM,I)

          IF(IP1.GT.N) GO TO 9
          IF(A(LM,I).EQ.0.0) GO TO 4
          DO 4 L=IP1,N
          A(LM,L)=A(LM,L)-A(1,L)*A(LM,I)
4         CONTINUE

9         A(LM,1)=A(LM,1)-A(1,I)*A(LM,I)
15        TC=C(1)
          DO 7 MN=1,N
          T=A(1,MN)
          IF(MN.GT.1) C(MN-1)=C(MN)
          DO 6 NO=2,N
6         A(NO-1,MN)=A(NO,MN)
7         A(N,MN)=T
          C(N)=TC
1         CONTINUE
          RETURN
          END
C***********************************************************************
          SUBROUTINE ELEM(IELEM)
C         COMMON/A1/CORD(NNOD,2),NNOD
          COMMON/A1/CORD(147,2),NNOD
C         COMMON/A2/KONECT(NELEM,3),NELEM
          COMMON/A2/KONECT(240,3),NELEM
          COMMON/A3/ELGK(3,3),ELF(3),LOCNOD(2),D(3,3),E(3)
          COMMON/A4/DXX,DXY,DYX,DYY,RETA,CST,XLAMD,Q,UX,UY,POR,DT,ALPH
C         COMMON/A5/CONC(NNOD)
          COMMON/A5/CONC(147)
C         COMMON/A6/NBOND,IBOND(NBOND,3)
          COMMON/A6/NBOND,IBOND(20,3)
          DIMENSION NODE(3),A(3,3),ELGP(3,3)
          DO 1 I=1,3
1         NODE(I)=KONECT(IELEM,I)
          B1=CORD(NODE(2),2)-CORD(NODE(3),2)
          B2=CORD(NODE(3),2)-CORD(NODE(1),2)
          B3=CORD(NODE(1),2)-CORD(NODE(2),2)
          C1=CORD(NODE(3),1)-CORD(NODE(2),1)
          C2=CORD(NODE(1),1)-CORD(NODE(3),1)
          C3=CORD(NODE(2),1)-CORD(NODE(1),1)
          EA=((C1*B3)-(C3*B1))/2.0
          EA=ABS(EA)
          DO 3 I=1,3
          ELF(I)=0.0
          DO 3 J=1,3
          ELGK(I,J)=0.0

          ELGP(I,J)=0.0
3         CONTINUE
C         TO CALCULATE ELEMENTAL MATRICES
          ELGK(1,1)=((DXX*B1**2)+(DXY*B1*C1)+(DYX*C1*B1)+(DYY*C1**2))/
         1(4.0*EA)+((UX*B1)+(UY*C1))/(6.0*POR)+(XLAMD*RETA*EA)/6.0
          ELGK(1,2)=((DXX*B1*B2)+(DXY*B1*C2)+(DYX*C1*B2)+(DYY*C1*C2))/
         1(4.0*EA)+((UX*B1)+(UY*C1))/(6.0*POR)+(XLAMD*RETA*EA)/12.0
          ELGK(1,3)=((DXX*B1*B3)+(DXY*B1*C3)+(DYX*C1*B3)+(DYY*C1*C3))/
         1(4.0*EA)+((UX*B1)+(UY*C1))/(6.0*POR)+(XLAMD*RETA*EA)/12.0
```

```
      ELGK(2,1)=((DXX*B2*B1)+(DXY*B2*C1)+(DYY*C2*C1)+(DYX*C2*B1))/
     1(4.0*EA)+((UX*B2)+(UY*C2))/(6.0*POR)+(XLAMD*RETA*EA)/12.0
      ELGK(2,2)=((DXX*B2**2)+(DXY*B2*C2)+(DYX*C2*B2)+(DYY*C2**2))/
     1(4.0*EA)+((UX*B2)+(UY*C2))/(6.0*POR)+(XLAMD*RETA*EA)/6.0
      ELGK(2,3)=((DXX*B2*B3)+(DXY*B2*C3)+(DYX*C2*B3)+(DYY*C2*C3))/
     1(4.0*EA)+((UX*B2)+(UY*C2))/(6.0*POR)+(XLAMD*RETA*EA)/12.0
      ELGK(3,1)=((DXX*B3*B1)+(DXY*B3*C1)+(DYX*C3*B1)+(DYY*C3*C1))/
     1(4.0*EA)+((UX*B3)+(UY*C3))/(6.0*POR)+(XLAMD*RETA*EA)/12.0
      ELGK(3,2)=((DXX*B3*B2)+(DXY*B3*C2)+(DYX*C3*B2)+(DYY*C3*C2))/
     1(4.0*EA)+((UX*B3)+(UY*C3))/(6.0*POR)+(XLAMD*RETA*EA)/12.0
      ELGK(3,3)=((DXX*B3**2)+(DXY*B3*C3)+(DYX*C3*B3)+(DYY*C3**2))/
     1(4.0*EA)+((UX*B3)+(UY*C3))/(6.0*POR)+(XLAMD*RETA*EA)/6.0
      ELGP(1,1)=(RETA*EA)/(6.0*DT)
      ELGP(1,2)=(RETA*EA)/(12.0*DT)
      ELGP(1,3)=(RETA*EA)/(12.0*DT)
      ELGP(2,1)=(RETA*EA)/(12.0*DT)
      ELGP(2,2)=(RETA*EA)/(6.0*DT)
      ELGP(2,3)=(RETA*EA)/(12.0*DT)
      ELGP(3,1)=(RETA*EA)/(12.0*DT)
      ELGP(3,2)=(RETA*EA)/(12.0*DT)
      ELGP(3,3)=(RETA*EA)/(6.0*DT)
      ELF(1)=(Q*CST*EA)/(3.0*POR)
      ELF(2)=(Q*CST*EA)/(3.0*POR)
      ELF(3)=(Q*CST*EA)/(3.0*POR)
C     CHECK FOR BOUNDARY ELEMENT
C     IBOND=ISARCH(12)
      IROW=0
401   IROW1=IROW+1
      DO 201 I2=IROW1,NBOND
      ICHECK=0
      IF(IELEM.NE.IBOND(I2,1)) GO TO 201
      ICHECK=1
      IROW=I2
      GO TO 202
201   CONTINUE
202   CONTINUE
      IF(ICHECK.EQ.0) GO TO 301
      INOD1=IBOND(IROW,2) ; JNOD1=IBOND(IROW,3)
      IF(INOD1.EQ.KONECT(IELEM,1)) LOCNOD(1)=1
      IF(INOD1.EQ.KONECT(IELEM,2)) LOCNOD(1)=2
      IF(INOD1.EQ.KONECT(IELEM,3)) LOCNOD(1)=3
      IF(JNOD1.EQ.KONECT(IELEM,1)) LOCNOD(2)=1
      IF(JNOD1.EQ.KONECT(IELEM,2)) LOCNOD(2)=2
      IF(JNOD1.EQ.KONECT(IELEM,3)) LOCNOD(2)=3
C     TYPE *,LOCNOD(1),LOCNOD(2),INOD1,JNOD1
      CALL SURFAC(INOD1,JNOD1)
      GO TO 401
301   CONTINUE
      TH=0.9
      DO 5 I=1,3
      DO 5 J=1,3
      A(I,J)=D(I,J)+(ELGP(I,J)-((1.0-TH)*ELGK(I,J)))
      ELGK(I,J)=(ELGP(I,J)+TH*(ELGK(I,J)))
5     CONTINUE
      DO 6 I=1,3
      DO 6 J=1,3
      ELF(I)=E(I)+ELF(I)+A(I,J)*CONC(KONECT(IELEM,J))
6     CONTINUE
      RETURN
      END
C*************************************************************************
      SUBROUTINE ASMBL
      COMMON/A1/CORD(147,2),NNOD
      COMMON/A2/KONECT(240,3),NELEM
      COMMON/A3/ELGK(3,3),ELF(3),LOCNOD(2),D(3,3),F(3)
      COMMON/A4/DXX,DXY,DYX,DYY,RETA,CSI,XLAMD,Q,UX,UY,POR,DT,ALPH
      COMMON/A5/CONC(147)
      COMMON/A6/NBOND,IBOND(20,3)
      COMMON/A7/GLGK(147,147),GLF(147)
      DO 1 I=1,NNOD
      GLF(I)=0.0
      DO 1 J=1,NNOD
      GLGK(I,J)=0.0
1     CONTINUE
      DO 2 I=1,NELEM
      IELEM=I
      CALL ELEM(IELEM)
      DO 2 J=1,3
      GLF(KONECT(IELEM,J))=GLF(KONECT(IELEM,J))+ELF(J)
      DO 2 K=1,3
      GLGK(KONECT(IELEM,J),KONECT(IELEM,K))=GLGK(KONECT(IELEM,J),
     1KONECT(IELEM,K))+ELGK(J,K)
2     CONTINUE
C     DO 71 I=1,6
C71   WRITE(20,*),(GLGK(I,J),J=1,6)
      RETURN
      END
```

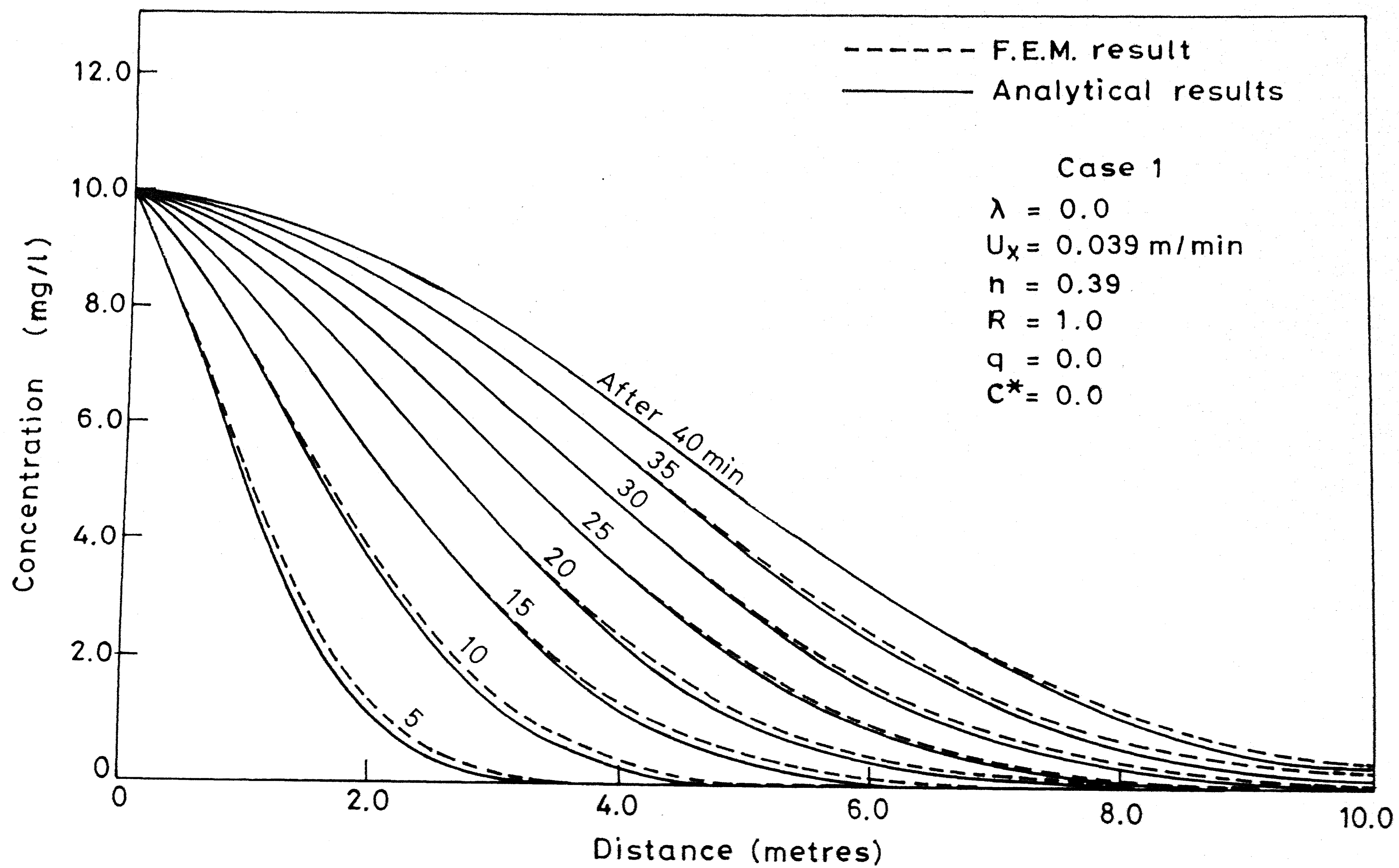


Fig. 4.1 Comparison of analytical results with F.E.M. results for linear elements, case 1.

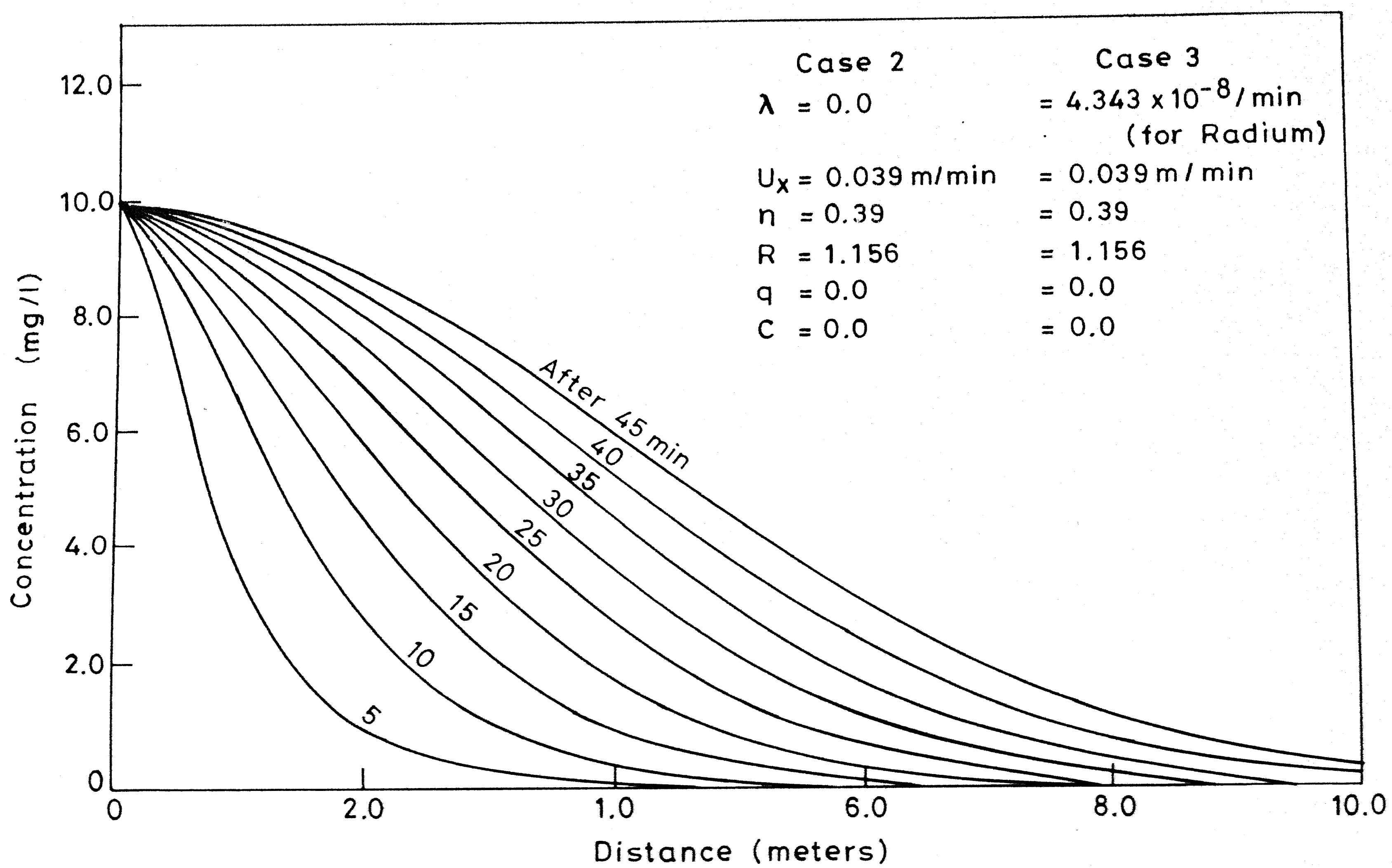


Fig. 4.2 F.E.M. results for case 2 and 3.

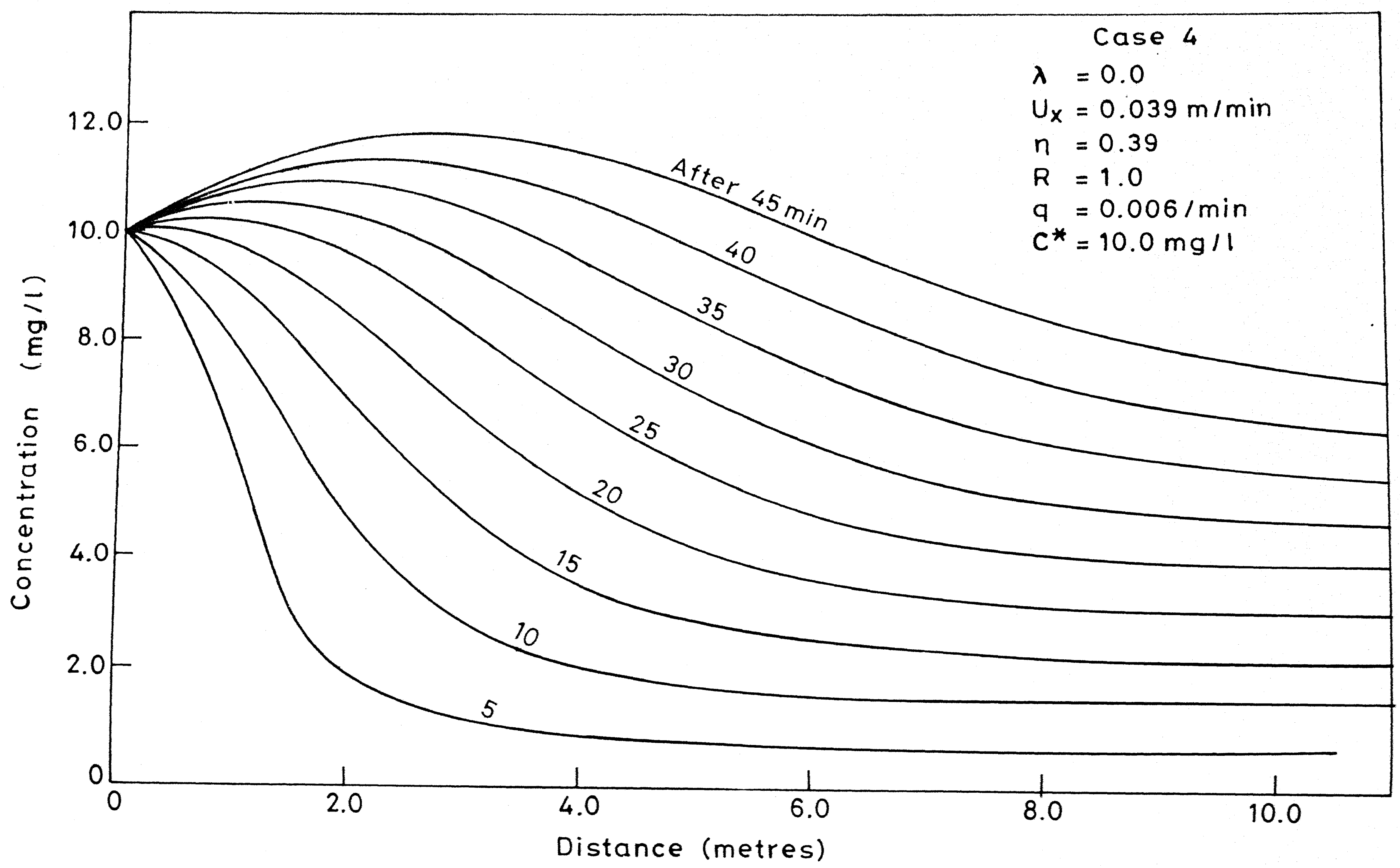


Fig. 4.3 F.E.M. results for case 4.

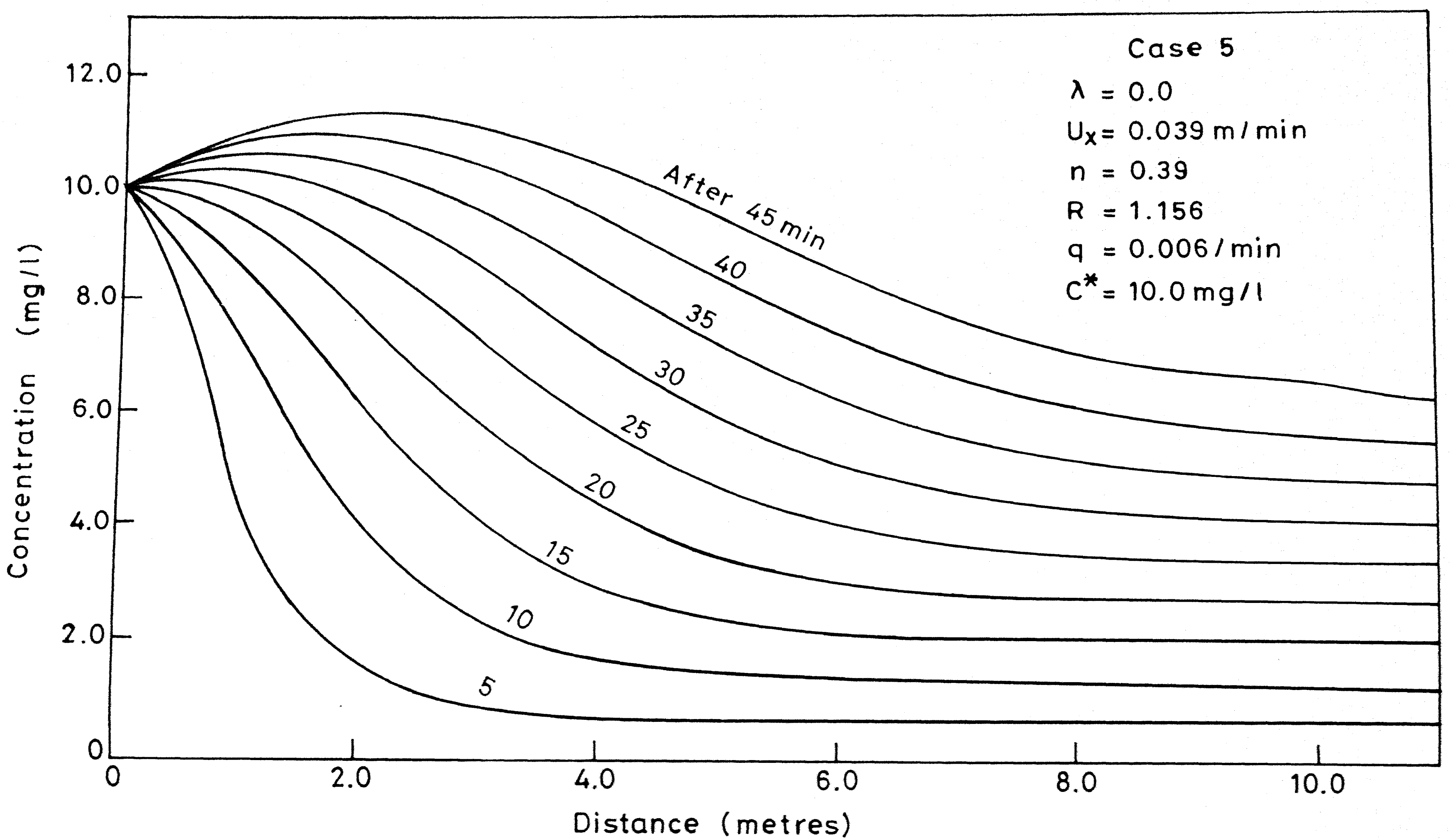


Fig. 4.4 F.E.M. results for case 5.

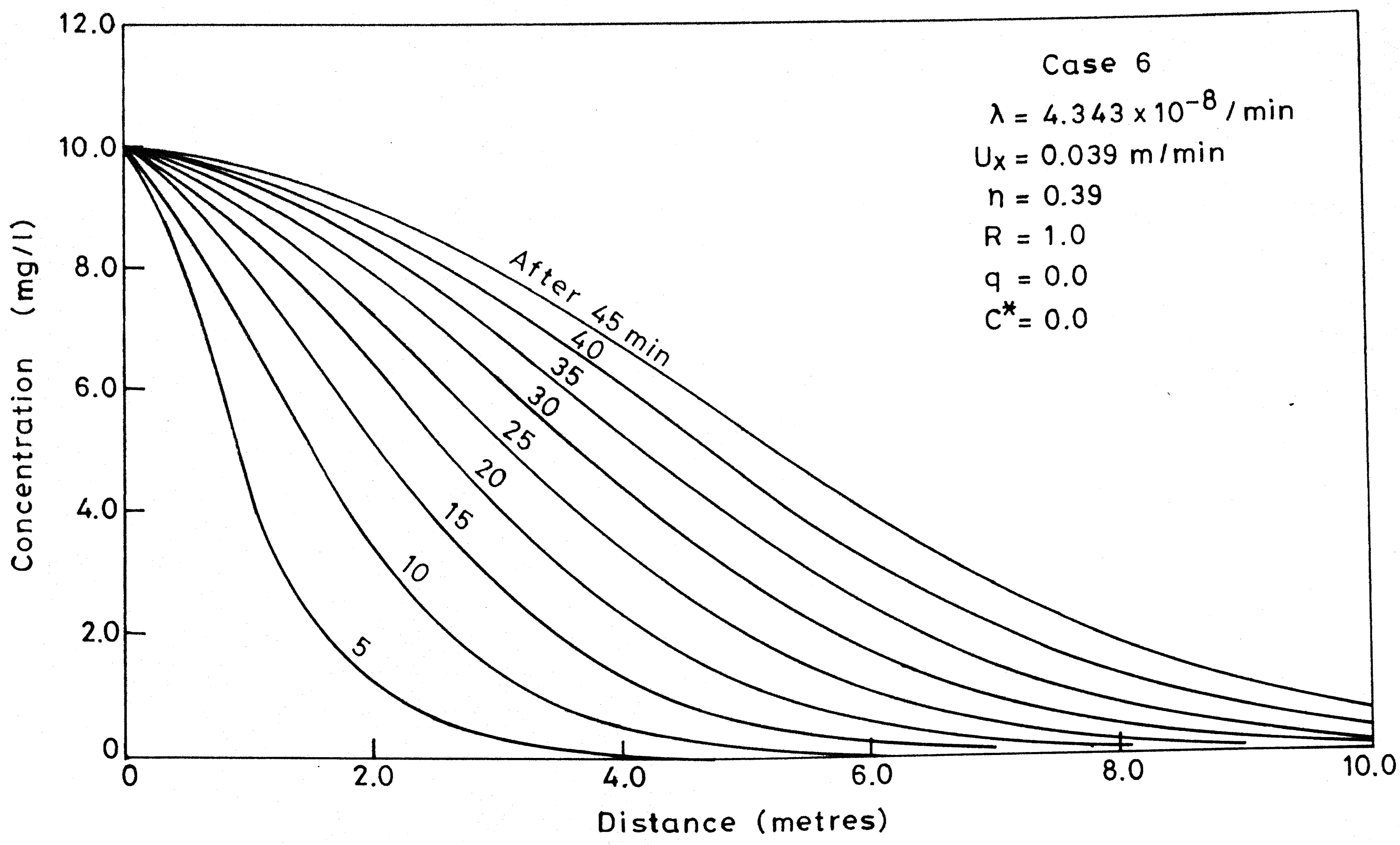


Fig. 4.5 F.E.M. results for case 6.

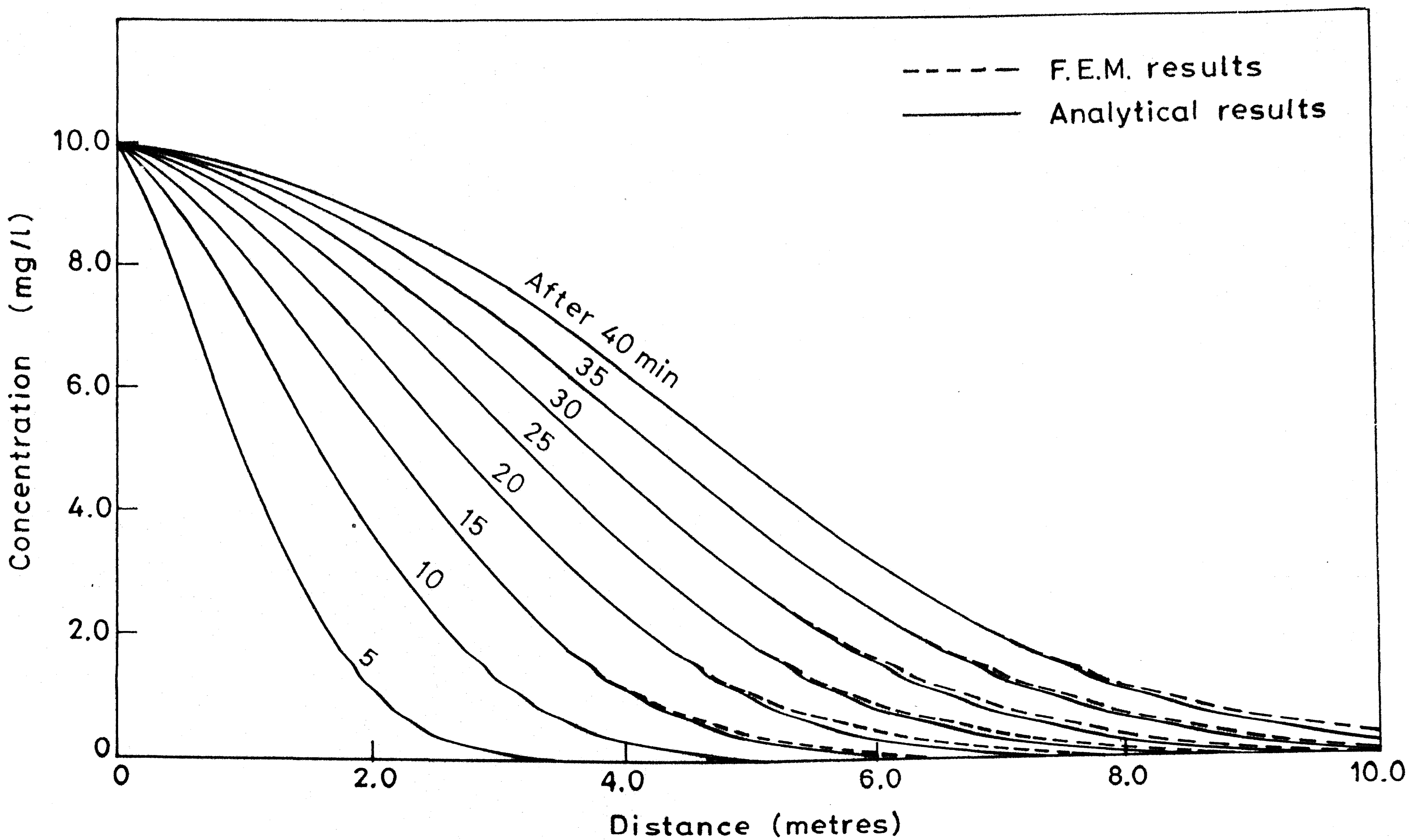


Fig. 4.6 Comparison of analytical results and F.E.M. results for quadratic case.

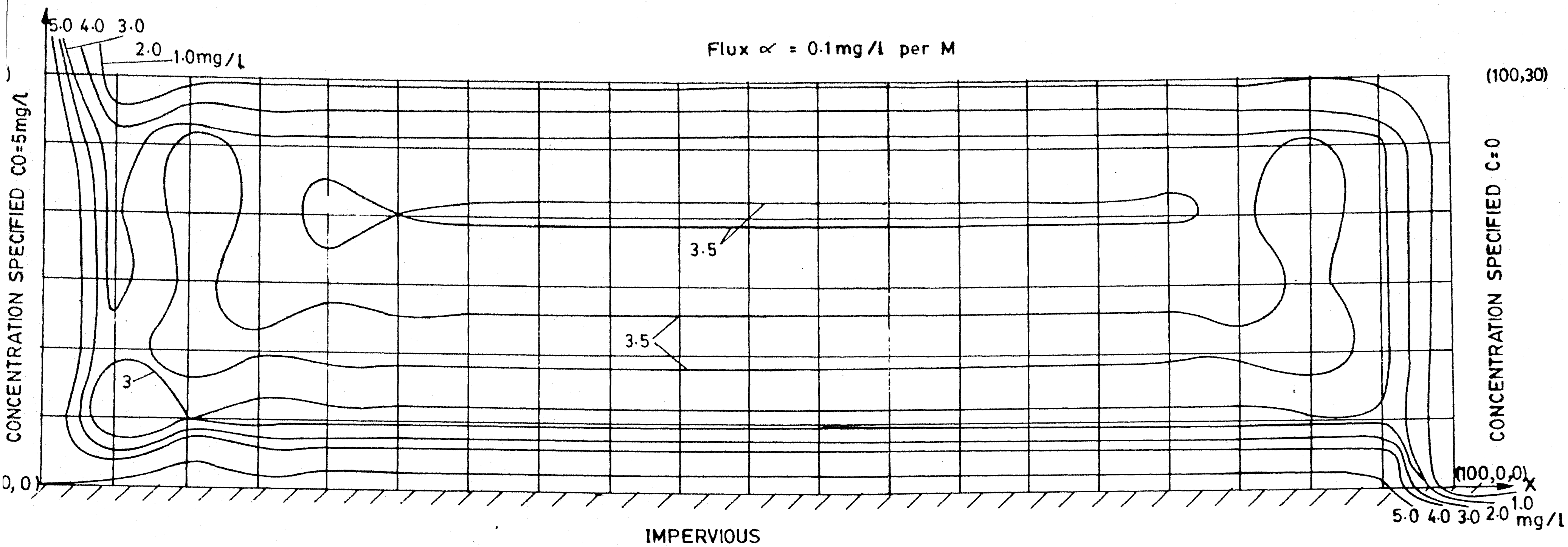


FIG. 4·7(a) Concentration contours for two dimensional case at t = 10 mins.

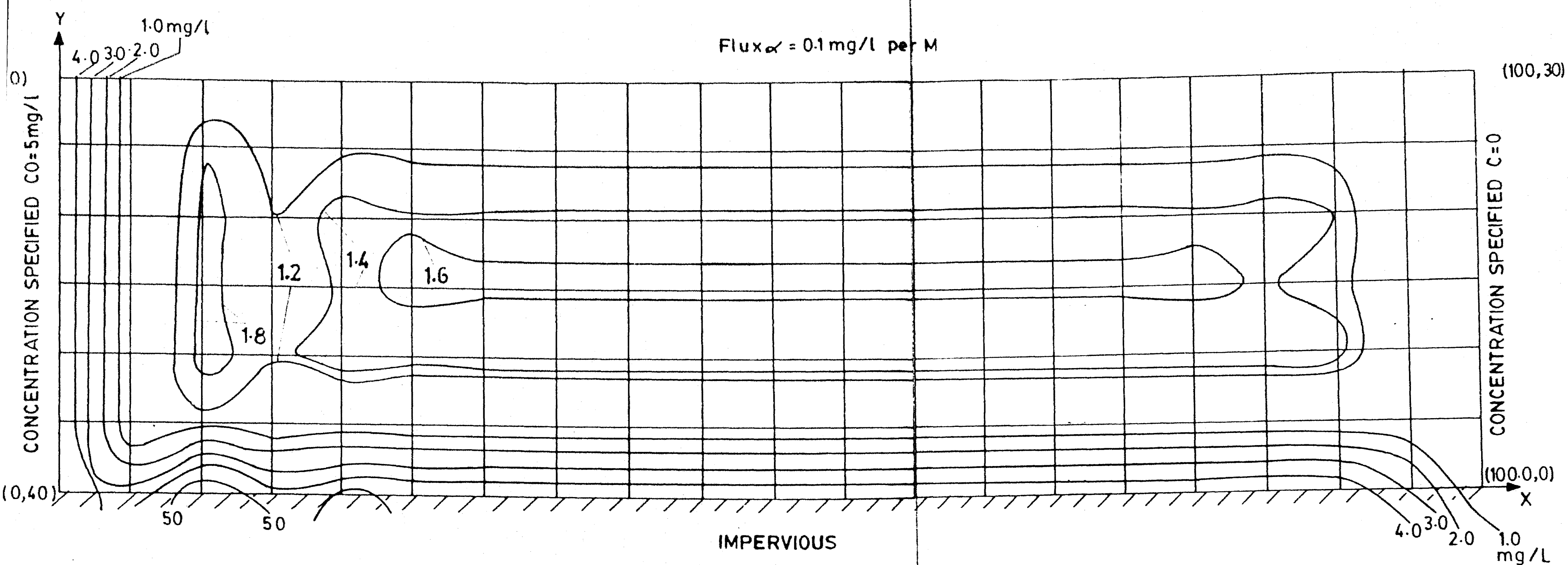


FIG. 4.7 (b) Concentration contours for two dimensional case at t = 25 mins

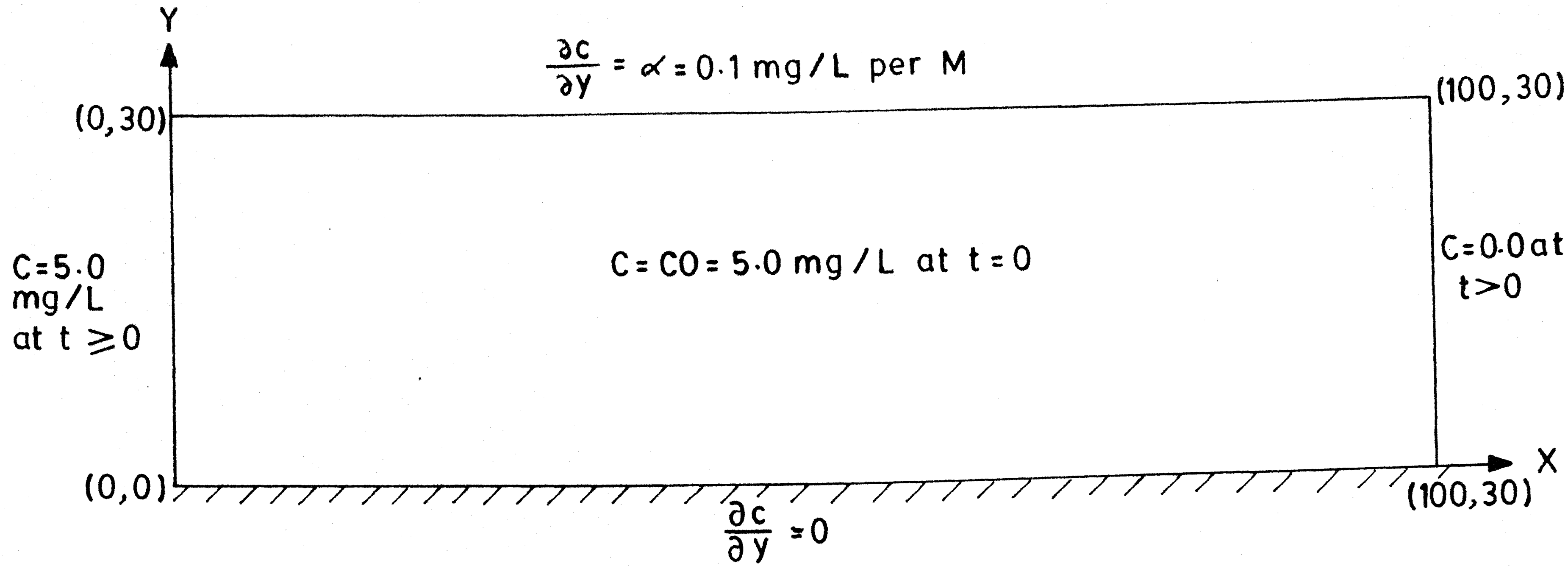


FIG. 4.8 A FIRST SET OF DOMAIN SHOWING BOUNDARY CONDITIONS

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